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Solving variational inequalities with a quadratic cut method: a primal-dual, Jacobian-free approach

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Abstract

We extend in two directions the Analytic Center, Cutting Plane Method for Variational Inequalities with quadratic cuts, ACCPM-VI(quadratic cuts), introduced by Denault and Goffin in 1998. First, we define a primal–dual method to find the analytic center at each iteration. Second, the Broyden–Fletcher–Goldfarb–Shanno Jacobian approximation, of quasi-Newton fame, is used in the definition of the cuts, making the algorithm applicable to problems without tractable Jacobians. The algorithm is tested on a variety of variational inequality problems, including one challenging problem of pricing the pollution permits put forward in the Kyoto Protocol.

Keywords: Variational inequalities; Analytic center cutting plane method; Quadratic cuts; Markal-macro model; Greenhouse gases; Emissions trading

1. Introduction

Finite-dimensional variational inequalities, and the closely related complementarity problems, have been a focus of renewed attention in the mathematical programming and operations research communities. The natural ability of variational inequalities to model equilibrium problems has led to numerous applications in the areas of transportation, economics, finance, environment, engineering, etc. The development of algorithms to solve variational inequalities has also been intense, and has

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assimilated many advances of other branches of mathematical programming, e.g. interior-point methods.

In this paper, the ACCPM-VI (quadratic cuts) approach of [1] is implemented in a primal-dual, infeasible setting; primal-dual methods, while more difficult to analyze, are robust and have a built-in centrality measure. Of great practical interest, we give promising results on the use of approximations of the Jacobian information that is required by the quadratic cut. The approximation is done with the BFGS matrix, in the spirit of quasi-Newton methods. The algorithm is admittedly heuristic, in that we do not provide a convergence proof; algorithms that drop cuts, as this one, are notoriously difficult to analyze.

The use of "quasi-Jacobian", temporary, quadratic cuts allows us to solve efficiently a particularly difficult variational inequality that arises in CO_2 emission permits trading (see [2]); this VI is such that the Jacobian of the associated mapping is not defined.

Following this introduction, Section 2 presents the generic ACCPM-VI (quadratic cuts) algorithm introduced in [1], while recalling some definitions and results on variational inequalities and analytic center. In Section 3, we derive our primal-dual method to locate an analytic center. We discuss in Section 4 the use of Jacobian proxies, and provide in Section 5 the results of our numerical experiments. We conclude in Section 6.

2. Solution of variational inequalities as convex feasibility problems: a quadratic cut approach

We begin, in Section 2.1, with a succinct overview of the literature on cutting plane approaches for variational inequalities. Then in Section 2.2, we introduce more formally the variational inequality, the convex feasibility problem, and the theorem that links them. Section 2.3 defines and motivates the quadratic cuts. Section 2.4 introduces the analytic center and other related concepts. Finally, in Section 2.5, we bring together linear cuts, quadratic cuts, and analytic centers in an algorithm for variational inequalities.

2.1. Review of cutting plane methods for variational inequalities

The ACCPM-VI algorithms (there are many versions) all use, in one way or another, the Analytic Center Cutting Plane Method, pioneered by Goffin and Vial (see the recent survey [3]) to solve Variational Inequality problems. The ACCPM, in turn, is fundamentally based on the interior point methods that originated in linear programming in the 1980's.

An ACCPM-VI approach is basically as follows. The variational inequality problem $VI(F, Y)$,

Find $y^* \in Y$ such that

$$F(y^*)^t(y - y^*) \geqslant 0 \quad \forall y \in Y$$

under the property of pseudo-monotonicity of its mapping F, can be written as a convex feasibility problem, i.e. one that comes with its own "cutting plane generation oracle" packaged in. This formulation was used by Goffin et al. [4] to solve the pseudomonotone $VI(F, Y)$: at the analytic center of a *localization set* known to contain the solution set of $VI(F, Y)$, a (linear) cut is generated, which separates the center from the solution set of $VI(F, Y)$. A complete implementation of the method

was described in [5], who use a primal–dual approach to find the analytic centers; the method was also extended to point-to-set mappings.

Later, quadratic cut approaches were devised, which make use of Jacobian information at the analytic center. In one category of methods, Lüthi and Büeler [6,7] and Mokhtarian and Goffin [8] derive algorithms that *accumulate* the quadratic cuts until a solution of $VI(F, Y)$ is found; they require the strong monotonicity of F. In a second category, Denault and Goffin [1] have suggested the use of quadratic cuts on a temporary basis, with the sole purpose of improving the location of the next cut. This approach, named "ACCPM-VI (quadratic cuts)" appears to be quite robust, and has even been advantageously applied to not strongly monotone problems (for example, see Section 5.3 below). Two algorithms are proposed in [1] to find the analytic centers, both working in the dual space (given the established terminology, the dual space here is the space in which Y lies).

2.2. Variational inequalities and convex feasibility problems

The variational inequality problem is defined as follows:

Definition 1. Let F be a continuous mapping from $\mathbb{R}^m$ into $\mathbb{R}^m$ and let Y be a nonempty subset of $\mathbb{R}^m$. Then the *variational inequality problem*, denoted $VI(F, Y)$, is to find a point $y^* \in Y$ such that

$$F(y^*)^t(y - y^*) \geqslant 0 \quad \forall y \in Y. \tag{1}$$

We will refer to the following properties of mappings:

Definition 2. Over a convex set Y, a mapping $F : \mathbb{R}^m \to \mathbb{R}^m$ is

- *monotone* if
$$(F(y_1) - F(y_2))^t(y_1 - y_2) \geqslant 0 \quad \forall y_1, y_2 \in Y;$$
- *strongly monotone with modulus* $\bar{\alpha}$ (or $\bar{\alpha}$-strongly monotone) if
$$(F(y_1) - F(y_2))^t(y_1 - y_2) \geqslant \bar{\alpha}\|y_1 - y_2\|^2 \quad \forall y_1, y_2 \in Y, \ \ y_1 \neq y_2;$$
- *pseudo-monotone* if
$$F(y_2)^t(y_1 - y_2) \geqslant 0 \Rightarrow F(y_1)^t(y_1 - y_2) \geqslant 0 \quad \forall y_1, y_2 \in Y.$$

We loosely refer to VIs defined with strongly monotone mappings, as highly monotone and we refer to VIs with monotone or pseudo-monotone mappings as having lower monotonicity. In fact, it is usually quite difficult to establish the "level of monotonicity" of a specific VI, such that unprecise statements such as "low monotonicity" is often the best one can do.

An algorithm for solving pseudo-monotone VIs as convex feasibility problems was given in [4]. A *convex feasibility problem* is defined by an oracle which, for any point $y \in \mathbb{R}^m$, either tells that the point belongs to an implicitly-defined, convex feasible set, and as such is a solution to the problem; or returns a hyperplane separating the point from the feasible set. The convex feasibility formulation of the VI relies on the following theorem due to Karamardian [9]:

Theorem 1. *Let Y be a nonempty, closed, convex subset of $\mathbb{R}^m$ and let F be a continuous, pseudomonotone mapping from Y into $\mathbb{R}^m$. Then y^* solves the $VI(F,Y)$ if and only if $y^* \in Y$ and*

$$F(y)^t(y - y^*) \geqslant 0 \quad \forall y \in Y. \tag{2}$$

Therefore, at any point $y_k \in Y$, the *linear cut* $F(y_k)^t(y_k - y) \geqslant 0$ defines a half-space

$$\{y \in \mathbb{R}^m \mid F(y_k)^t(y - y_k) \leqslant 0\} \tag{3}$$

which contains the solution set of $VI(F,Y)$ and on whose border y_k lies.

Quadratic cuts are defined next, and are then integrated in a convex feasibility, quadratic cut formulation in Section 2.5.

2.3. Quadratic cuts

While Theorem 1 justifies linear cuts, it is also possible to define *quadratic cuts* when F is differentiable (Jacobian-free quadratic cuts are also discussed in Section 4). Since the cut is generated at some point $y_k \in Y$ and is meant to lie in the half-space (3), a natural family of quadratic cuts, parameterized by $\gamma \geqslant 0$, is

$$Q_\gamma(y_k) \triangleq \{y \in \mathbb{R}^m \mid \gamma(y - y_k)^t \nabla_k (y - y_k) + F(y_k)^t(y - y_k) \leqslant 0\} \tag{4}$$

where ∇_k is some positive definite matrix, eventually based on the Jacobian at y_k, when it exists. Clearly, we obtain the linear cut (3) for the boundary case $\gamma = 0$. The more interesting quadratic cut with

$$\nabla_k \triangleq \frac{\nabla F(y_k) + \nabla F(y_k)^t}{2} \tag{5}$$

and $\gamma = \frac{1}{2}$ is motivated in [1]. This choice of ∇_k as the symmetrized Jacobian simply underlines that only the symmetric part of ∇_k plays a role in the cut; more importantly, our implicit assumption here is that F is α-strongly monotone, since we assumed that ∇_k is a positive definite matrix. This quadratic cut is the one used in this paper, which we denote as

$$Q(y_k) \triangleq \left\{ y \in \mathbb{R}^m \mid (y - y_k)^t \frac{\nabla_k}{2} (y - y_k) + F(y_k)^t(y - y_k) \leqslant 0 \right\}. \tag{6}$$

The cut $Q(y_k)$ defines an ellipsoid, on the border of which y_k lies.

It is very important to notice that without a result analog to Theorem 1, there is no guarantee that a cut (6) even contains the solution(s) of (1): we call such cuts *unsafe*.

Under the assumption of α-strong monotonicity, it is possible to devise *safe* cuts that never leave the solution out, and which, incidently, are independent of the Jacobian, see Lüthi and Büeler, [6,7]. Also, under the same assumption of α-strong monotonicity, some members of the family of cuts $Q_\gamma(y_k)$ are safe cuts: any ellipsoid $Q_\gamma(y_k)$ with γ such that $\gamma \nabla_k \preccurlyeq \alpha I$, will not cut off the solution point[3]. The proof is easy to develop with the results of [6].

[3] The sign $\preccurlyeq$ denotes the Loewner matrix ordering: $M \preccurlyeq N$ if $N - M$ is positive semi-definite.

Nevertheless, with the goal of a practical algorithm in mind, we build our approach on *unsafe* cuts, not safe ones. The rationale is simple: it is in most examples difficult to evaluate the monotonicity of a mapping, let alone it level α of strong-monotonicity. To use safe cuts, one must then choose between a quadratic cut with a conservative, very small value of γ, making the cut almost linear; or a cut with a not-so-small γ, at the risk of including "safe" cuts that are not so. Our approach to managing unsafe cuts is explained in Section 2.5.

2.4. Analytic centers and Dikin ellipsoids

Since their introduction, analytic centers have been used in a wide variety of contexts; see [3] for several examples.

Although they were originally defined for polyhedral sets, the definition is easily extended, as described in Section 2.4.2.

2.4.1. Analytic centers of polyhedral sets and Dikin ellipsoids

Definition 3. Consider the polyhedral set

$$W = \{y \mid A^t y \leqslant c\}$$

and the associated *dual potential function*

$$\sum_i \ln(c_i - a_i^t y)$$

where the index i is used to denote the components of c and the rows a_i^t of A^t.

The *analytic center* y^c of W is defined as the point maximizing the following potential function over the interior of W:

$$y^c = \arg\max_{y \in \operatorname{int} W} \left(\sum_i \ln(c_i - a_i^t y) \right).$$

This potential function is called "dual"; one can alternatively define the analytic center with the primal potential function or the primal-dual one, obtaining in all cases the same point. It is well known that if W is bounded, the center y^c is unique. Writing out the first-order optimality conditions for the equivalent mathematical program

$$\begin{aligned} \underset{y,s}{\text{maximize}} \quad & \sum_i \ln s_i \\ \text{subject to} \quad & A^t y + s = c, \\ & s > 0, \end{aligned}$$

we obtain the now-classical equations

$$Ax = 0, \tag{7}$$

$$A^t y + s = c, \tag{8}$$

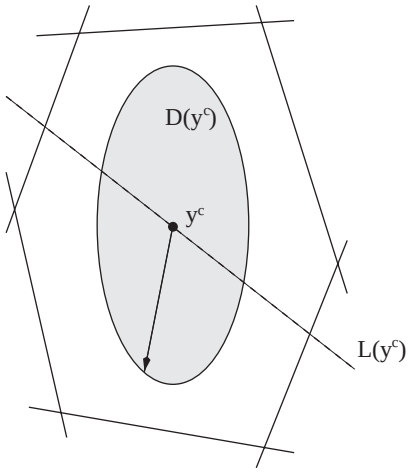

Fig. 1. Dikin ellipse and Dikin direction of some polyhedral set.

$$Xs = e, \tag{9}$$

$$x, s > 0, \tag{10}$$

where we follow the notational usage: X is the diagonal matrix whose non-zeros are given by x, and e is a vector of ones of appropriate dimension.

Let us also define the *ellipsoid of Dikin at* $\bar{y}$

$$D(\bar{y}) = \{y \mid (y - \bar{y})^t (A\bar{S}^{-2}A^t)(y - \bar{y}) \leqslant 1\}$$

where $\bar{s} = c - A^t\bar{y}$ as in the above equations. See [10] for reference, and Fig. 1 for an illustration of the ellipsoid at the analytic center y^c This ellipsoid can be defined at any point $\bar{y} \in \text{int}(W)$, and it is always inscribed in W, i.e. $D(\bar{y}) \subset W$; a proof is given in [11].

Finally, for the mapping $F : \mathbb{R}^m \to \mathbb{R}^m$ and the hyperplane $\{y \mid F(\bar{y})^t y = F(\bar{y})^t \bar{y}\}$, the point in $D(\bar{y})$ that is the farthest from the hyperplane is

$$\bar{y} - \frac{1}{\sqrt{F(\bar{y})^t (A\bar{S}^{-2}A^t)^{-1} F(\bar{y})}} (A\bar{S}^{-2}A^t)^{-1} F(\bar{y}).$$

The second term is called *Dikin direction*. See the arrow in Fig. 1, where the hyperplane is denoted $L(y^c)$.

2.4.2. Analytic centers of polyhedral-quadratic sets

When considering sets that comprise linear inequalities as well as a quadratic inequality, the definition of the analytic center must be adapted as follows.

If we consider the polyhedral-quadratic set

$$W \cap Q(y_k) = \{y \in \mathbb{R}^m | A^t y \leqslant c\} \cap \{y \in \mathbb{R}^m | (1/2)(y - y_k)^t \nabla_k (y - y_k) + F(y_k)^t (y - y_k) \leqslant 0\}$$

and we define corresponding slack variables

$$s \triangleq c - A^t y \tag{11}$$

$$s_q \triangleq -(y - y_k)^t \frac{\nabla_k}{2}(y - y_k) - F(y_k)^t(y - y_k) \tag{12}$$

then the analytic center of $W \cap Q(y_k)$ can be defined as the point maximizing the appropriate potential function over the interior of $W \cap Q(y_k)$:

$$y^c = \arg \max_{y \in \mathrm{int}(W \cap Q(y_k))} \left(\ln s_q + \sum_i \ln(c_i - a_i^t y) \right)$$

where as before i denotes the components of c and the rows a_i^t of the $n \times m$ matrix A^t. The optimality conditions for this maximization problem are

$$\begin{aligned}
&Ax + x_q(\nabla_k(y - y_k) + F(y_k)) = 0,\\
&A^t y + s = c,\\
&(y - y_k)^t \frac{\nabla_k}{2}(y - y_k) + F(y_k)^t(y - y_k) + s_q = 0,\\
&Xs = e,\\
&x_q s_q = 1,\\
&x, s, x_q, s_q > 0.
\end{aligned} \tag{13}$$

The primal variables $x \in \mathbb{R}^n_+$ and $x_q \in \mathbb{R}_+$ are, respectively, associated with the linear cuts and the quadratic cut. It is usual to refer to the first equation as the primal feasibility constraint, to the second and third equations as the dual feasibility constraints, to the fourth and fifth equations as the centrality constraints.

2.5. A quadratic cut algorithm

As discussed in Section 2.2, a convex feasibility formulation of the variational inequality problem was introduced by [4], whose approach uses linear cutting planes and analytic centers. Fundamentally, a cut is introduced at the center of a *set of localization*, known to contain the solution(s). This cut separates the set of localization in two parts; under some qualification of F, one of the two parts is known to contain the solution set. The size of the set of localization can then be decreased; the analytic center of the reduced set is found, and the process repeated.

We recall in this section a method, introduced in [1] which shares the "cutting planes and analytic centers" foundation, but that uses quadratic cuts to improve the speed of convergence.

Recall that the Jacobian-based quadratic cut $Q(y_k)$ given in (6) can suffer the major drawback of possibly cutting off solution points. To avoid leaving a solution point irremediably out of reach, quadratic cuts are introduced on a *temporary* basis only: a cut $Q(y_k)$ is kept only until the next analytic center is found. At that point, the quadratic cut is abandoned and replaced by its corresponding, safer, linear cut.

A stopping criterion is required for the algorithm, and to this end we recall the following:

Definition 4. The *primal gap function* g associated with $VI(F, Y)$ and $y \in Y$ is defined as

$$g(y) = \inf_{z \in Y} F(y)^t (z - y).$$

Clearly, $g(y)$ is bounded above by 0, with the solution $z = y$. The primal gap is often used as stopping criterion, given that it is 0 if and only if y is a solution of $VI(F, Y)$ (see [12]); and also that for a compact, polyhedral set Y, $g(y)$ can be computed easily using standard linear programming approaches. In all our numerical results, we use a "relative" gap, defined with $F(y)/\|F(y)\|$ instead of $F(y)$.

A basic description of the algorithm is then as follows:

ALGORITHM ACCPM-VI (QUADRATIC CUTS)
Step 0: *Initialization*
Set $k = 0$, $Y_0 = Y$, and y_0 the analytic center of Y_0.
Step 1: *Termination criterion*
If the primal gap $g(y_k) \geqslant -\varepsilon$ then stop.
Step 2: *New cut*
Compute cut $(y - y_k)^t \frac{\nabla_k}{2}(y - y_k) + F(y_k)^t (y - y_k) \leqslant 0$.
Step 3: *Analytic center*
Find an approximate analytic center y_{k+1} of $Y_k \cap \{y : (y - y_k)^t \frac{\nabla_k}{2}(y - y_k) + F(y_k)^t (y - y_k) \leqslant 0\}$
Step 4: *Localization set update*
Set $Y_{k+1} := Y_k \cap \{y : F(y_k)^t y_k \geqslant F(y_k)^t y\}$
$k := k + 1$
Return to Step 1.

Step 1 consists of evaluating the primal gap defined earlier; this is the same criterion that was used in ACCPM-VI (linear cuts). Step 2 introduces the quadratic cut, which basically corresponds to a function evaluation and a Jacobian evaluation. Step 3 will be discussed in the next section; it is necessary to both define the linear-quadratic analytic center and give a method to find it. It is very important to realize that in Step 4, the cut used in the update is not the quadratic cut but its corresponding linear cut: in other words, the quadratic cut is abandoned and the corresponding linear cut simultaneously introduced. [4]

The crucial difficulty of the algorithm described above is to find, from a current analytic center, the next one. In the next section, we discuss a primal–dual, heuristic approach to solve this problem.

3. Primal–dual updating and recentering steps to the next analytic center

We describe here a primal–dual method for computing the next analytic center y_{k+1}, that of $Y_k \cap Q(y_k)$, when the quadratic cut $Q(y_k)$ is introduced at the current point y_k. More than one step may be necessary to reach y_{k+1} from y_k, and it is useful to distinguish the first step out of y_k,

[4] Note that although we routinely write $Y_k = \{y \mid A^t y \leqslant c\}$ for the sake of notational simplicity, A and c grow at each iteration, since a linear cut is added, and are indeed dependent on k.

called the *updating step*, from the following ones, called *centering steps*. The distinction is needed because of a special difficulty with the updating step: since y_k lies *on* the cut, the corresponding slack value is necessarily 0, thus infeasible with respect to the positivity constraints. This difficulty is encountered whether the cut be quadratic as here, or linear, as in [4,5].

Pure dual steps were derived in [1] for the same problem. One drawback of dual methods, is that the computation of the centrality measure, used to evaluate whether an approximate center is close enough to the actual analytic center, requires the computation of the centering step itself. This overhead being incurred in any case, at least one centering step is taken for every cut, irrespective of the quality of the center after the updating step. Primal-dual approaches come with a built-in centrality measure that requires no extra computation, and in many cases, the single updating step is sufficient to obtain an approximate center.

3.1. The primal–dual updating step

Fundamentally, initial values for the variables (y, s, x, s_q, x_q) are required, to start a Newton method on the equations of (13); these values should fulfill the positivity constraints of (13). To handle this "first step out of y_k" difficulty, the primal–dual linear cut approaches of [4,5] introduce a positive slack value for the new cut, even if this destroys the primal and dual feasibility; this positive value can be chosen analytically to ensure that a (full) Newton step will preserve all the positivity constraints. In a quadratic cut, it is more difficult to do so for lack of provably good values for the variables s_q and x_q associated to the new cut.

As much as possible, our initial value for s_q should be close to its desired value, i.e. the slack of the quadratic cut at the next analytic center. We recall the following heuristic approach to set the initial value of s_q, which was introduced in [1]. Two linesearches are performed from y_k, with the potential

$$\ln s_q + \sum_i \ln(c_i - a_i^t y)$$

as criterion. The two directions in question are (1) the straight line from y_k to the center of the quadratic cut ellipsoid $Q(y_k)$, and (2) the Dikin direction. Whichever linesearch is the most successful in finding an approximate center will have its corresponding slack as the initial slack value. The directions are illustrated in Figs. 2 and 3.

The rationale of the heuristic is as follows. If the quadratic cut ellipsoid is small relative to the Dikin ellipsoid, then the next analytic center y_{k+1} is likely to be close to the center of $Q(y_k)$, and the first linesearch will return a point relatively close to y_{k+1}. If the quadratic cut ellipsoid is large compared to the Dikin ellipsoid, the quadratic cut adds little more than the corresponding linear cut $F(y_k)^t(y - y_k) \leqslant 0$. Given that in the *linear cut* framework, i.e. that of [5] where a linear cut is introduced at y_k, the Dikin direction is the Newton direction towards the next analytic center y_{k+1}, it can be expected that the second linesearch will be relatively successful. In this second case, note that there is a point on the Dikin direction that is in the radius of quadratic convergence for the Newton method underlying the centering steps of the next section (see [13]).

Using the best result of the two linesearches would hopefully yield an reasonable approximation of the next analytic center, and so a reasonable initial value for s_q. The initial value of x_q is simply taken to be $1/s_q$, as we know that $x_q = 1/s_q$ holds at the analytic center.

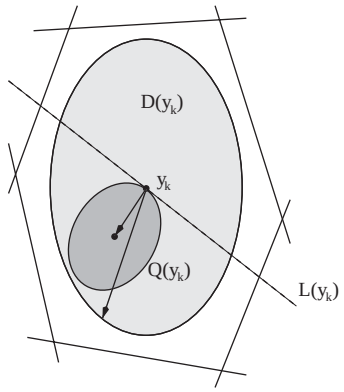

Fig. 2. The two search directions; case 1.

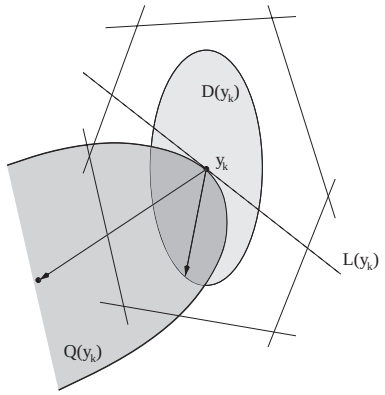

Fig. 3. The two search directions; case 2.

Applying Newton's method to the set of equations (13) we obtain a first step out of y_k. Our approach is primal-dual so that in fact we derive steps for all variables: y, s, x, s_q and x_q. Some remarks are in order, concerning the starting point which we denote as $(y_s, s_s, x_s, s_{q_s}, x_{q_s})$. First, notice that, after the computation of the point $(y_k, s_k, x_k, s_{q_k}, x_{q_k})$, (i.e. the previous analytic center as well as the values of its corresponding variables), one linear inequality (a cut) has been added to Y_{k-1} to define Y_k. This was the linear cut replacing the abandoned quadratic cut. As a consequence, s_s and x_s have one more component each than s_k and x_k. The starting values s_s and x_s are then set, with their "extra" components, so that on one hand, the linear dual feasibility condition holds, and on the other hand, the centrality is not disturbed:

$$s_s = \begin{bmatrix} s_k \\ F(y_{k-1})^t(y_{k-1} - y_k) \end{bmatrix}, \qquad x_s = \begin{bmatrix} x_k \\ \dfrac{1}{F(y_{k-1})^t(y_{k-1} - y_k)} \end{bmatrix}$$

The starting values s_{q_s} and x_{q_s} are determined by the procedure described at the beginning of this section. Finally, the initial value y_s is simply the current point, y_k.

Using this starting point, we obtain the following equations defining the step $(\mathrm{d}y, \mathrm{d}s, \mathrm{d}x, \mathrm{d}s_q, \mathrm{d}x_q)$:

$$A\mathrm{d}x + F(y_k)\,\mathrm{d}x_q + x_{q_s}\nabla_k\,\mathrm{d}y = -Ax_s - x_{q_s}F(y_k), \tag{14}$$

$$A^t\,\mathrm{d}y + \mathrm{d}s = -Ay_s - s_s + c = 0, \tag{15}$$

$$F(y_k)^t\mathrm{d}y + \mathrm{d}s_q = -s_{q_s}, \tag{16}$$

$$S_s\,\mathrm{d}x + X_s\,\mathrm{d}s = \delta, \tag{17}$$

$$s_{q_s}\,\mathrm{d}x_q + x_{q_s}\,\mathrm{d}s_q = 0, \tag{18}$$

where $\delta \triangleq e - X_s s_s$. The right handside term in (15) is a consequence of dual feasibility of (y_s, s_s). In (17), δ is *not* zero, which explicitly accounts for the inaccuracy in the centering of the previous center, y_k.

Rearranging these equations, and using the fact that, by our decision, $x_{q_s} = 1/s_{q_s}$, we obtain the following step:

$$\mathrm{d}y = -\Delta^{-1}\left(AS_s^{-1}e + \frac{2}{s_{q_s}}F(y_k)\right), \tag{19}$$

$$\mathrm{d}s = -A^t\,\mathrm{d}y, \tag{20}$$

$$\mathrm{d}s_q = -s_{q_s} - F(y_k)^t\,\mathrm{d}y, \tag{21}$$

$$\mathrm{d}x = S_s^{-1}(\delta - X_s\,\mathrm{d}s), \tag{22}$$

$$\mathrm{d}x_q = \frac{-\mathrm{d}s_q}{s_{q_s}^2}, \tag{23}$$

where Δ is defined as

$$\Delta \triangleq AS_s^{-1}X_sA^t + \frac{1}{s_{q_s}^2}F(y_k)F(y_k)^t + \frac{1}{s_{q_s}}\nabla_k.$$

Thus written, the step can clearly be seen as parameterized by the one-dimensional parameter s_{q_s}. Notice also that this step preserves dual feasibility since

$$A^t(y + \mathrm{d}y) + s + \mathrm{d}s = A^ty + s + A^t\,\mathrm{d}y - A^t\,\mathrm{d}y = 0.$$

If after the step, the centering level of the new point in the Euclidian norm

$$\left\|\begin{bmatrix}\mathrm{diag}(x_s + \mathrm{d}x)\cdot(s_s + \mathrm{d}s) - e\\ (x_{q_s} + \mathrm{d}x_q)\cdot(s_{q_s}\mathrm{d}s_q) - 1\end{bmatrix}\right\|_2 \tag{24}$$

is considered sufficient, then $y + \mathrm{d}y$ is taken as the new approximate center y_{k+1}. Otherwise, one or more *centering steps* are required; these are described in the following section.

3.2. Primal–dual centering steps

Let us denote by $y^+, s^+, x^+, s_q^+, x_q^+$ the result of the updating step, i.e.

$$
\begin{aligned}
y^+ &= y_s + \mathrm{d}y,\\
s^+ &= s_s + \mathrm{d}s,\\
x^+ &= x_s + \mathrm{d}x,\\
s_q^+ &= s_{q_s} + \mathrm{d}s_q,\\
x_q^+ &= x_{q_s} + \mathrm{d}x_q.
\end{aligned}
$$

We again apply Newton's method to the system of equations (13), using this time $(y^+, s^+, x^+, s_q^+, x_q^+)$ as starting point. We obtain

$$
\begin{aligned}
&A\,\mathrm{d}x + (\nabla_k(y^+ - y_k) + F(y_k))\,\mathrm{d}x_q + x_q^+\nabla_k\,\mathrm{d}y = -Ax^+ - x_q^+(\nabla_k(y^+ - y_k) + F(y_k)),\\
&A^t\,\mathrm{d}y + \mathrm{d}s = -Ay^+ - s^+ + c = 0,\\
&(\nabla_k(y^+ - y_k) + F(y_k))^t\,\mathrm{d}y + \mathrm{d}s_q = -q^2 - F(y_k)^t(y^+ - y_k) - s_q^+,\\
&S^+\mathrm{d}x + X^+\mathrm{d}s = \delta,\\
&s_q^+\mathrm{d}x_q + x_q^+\mathrm{d}s_q = 1 - s_q^+x_q^+,
\end{aligned}
$$

where we have used $\delta \triangleq e - X^+s^+$ and $q^2 \triangleq \frac{1}{2}(y^+ - y_k)^t\nabla_k(y^+ - y_k)$. These equations yield the *centering step*

$$
\begin{aligned}
\mathrm{d}y &= -(\Delta^+)^{-1}\left(AS_s^{-1}e + \left(\frac{1}{s_q^+} + x_q^+ + q^2 + F(y_k)^t(y^+ - y_k)\right)(\nabla_k(y^+ - y_k) + F(y_k))\right)\\
\mathrm{d}s &= -A^t\,\mathrm{d}y\\
\mathrm{d}s_q &= -s_q^+ - q^2 - F(y_k)^t((y^+ - y_k) - (2\nabla_k(y^+ - y_k) + F(y_k))\,\mathrm{d}y,\\
\mathrm{d}x &= (S^+)^{-1}(\delta - X^+\,\mathrm{d}s)\\
\mathrm{d}x_q &= \frac{1 - x_q^+\,\mathrm{d}s_q}{s_q^+}
\end{aligned}
$$

where Δ^+ is defined as

$$
\Delta^+ = A(S^+)^{-1}X^+A^t + \frac{x_q^+}{s_q^+}(\nabla_k(y^+ - y_k) + F(y_k))(\nabla_k(y^+ - y_k) + F(y_k))^t + x_q^+\nabla_k.
$$

Again, this step preserves the dual feasibility. The centering measure is again (24) and centering steps can be taken until the desired level of centering is reached.

4. Jacobian matrix approximations

Faced with an algorithm that uses derivative information (the Jacobian ∇F), one asks if it is not possible to keep the spirit of the method while avoiding the derivatives evaluations. The answer, often, is yes; in optimization, the idea led to the quasi-Newton methods. In our case, the use of Jacobian approximations based on mapping evaluations can also be fruitful.

Drawing from well-established optimization theory, we use a Broyden–Fletcher–Goldfarb–Shanno (BFGS) matrix for the Jacobian approximation. The BFGS-type approximation is a symmetric matrix which is updated by a rank-two correction whenever a new quadratic cut is generated. Importantly, the BFGS scheme is built to preserve positive definiteness of the approximation matrix, under a condition discussed below.

Defining the notation $y_\Delta := y_{k+1} - y_k$ and $F_\Delta := F(y_{k+1}) - F(y_k)$, the BFGS Jacobian approximation for $\nabla F(y_{k+1})$ is

$$J_{k+1} = J_k + \frac{F_\Delta F_\Delta^t}{F_\Delta^t y_\Delta} - \frac{J_k y_\Delta y_\Delta^t J_k}{y_\Delta^t J_k y_\Delta}.$$

The updating process is usually initiated with the identity matrix. Under the strict monotonicity of F, positive definiteness is preserved: if J_k is positive definite, then so is J_{k+1}. Indeed, for any $z \neq 0$,

$$\begin{aligned} z^t J_{k+1} z &= z^t J_k z + \frac{z^t F_\Delta F_\Delta^t z}{F_\Delta^t y_\Delta} - \frac{z^t J_k y_\Delta y_\Delta^t J_k z}{y_\Delta^t J_k y_\Delta} \\ &= \frac{(z^t J_k z)(y_\Delta^t J_k y_\Delta) - (y_\Delta^t J_k z)^2}{y_\Delta^t J_k y_\Delta} + \frac{(F_\Delta^t z)^2}{F_\Delta^t y_\Delta}. \end{aligned}$$

The first term of the right-hand side is non-negative by the Cauchy–Schwarz inequality and the positive-definiteness of J_k; the second term is non-negative because of the monotonicity assumption. Also, the two terms cannot vanish at the same time: the first vanishes only if $z = \lambda y_\Delta$ for some $\lambda \in \mathbb{R}$ ($\lambda \neq 0$), and in that case $F_\Delta^t z = \lambda F_\Delta^t y_\Delta$, which is nonzero by strict monotonicity.

In some cases, an analysis of the approximation's quality can be carried out. For example, Quasi-Newton updates such as the BFGS are built upon the concept of *finite-step convergence*: if F is a symmetric linear mapping, then the updates converge to the exact Jacobian in a finite number of steps. Unfortunately, this finite convergence is lost for nonlinear mappings. Furthermore, this property relies on $F(y_{k+1})(y_{k+1} - y_k) = 0$, which will not hold in our algorithm. On the other hand, note that as a sum of symmetric matrices, J_{k+1} is symmetric, and thus approximates only the symmetric part of the Jacobian. Nothing is lost here for our algorithm, since the quadratic cut only uses the symmetric part of the Jacobian in any case.

The scaling of the updates (λJ_k for some $\lambda \in \mathbb{R}^+$) is a common improvement for quasi-Newton methods, and this is the last point we discuss in this section. In optimization, scaling is motivated by an argument emphasizing an improvement of the solution at each iteration, as opposed to some

global convergence over several iterations (see, for example, Luenberger [14]). The argument applies to the idealized case of strictly convex, unconstrained quadratic minimization, with exact optimal steplengths available; scaling is however also applied to the more general cases (nonlinear but non quadratic functions, inexact linesearches), usually with great benefit. The same is true with our algorithm, namely, the argument from optimization applies to an idealized VI problem, but scaling can bring benefits in the general VI case. Indeed, consider a problem $VI(F, Y)$ where F is a linear mapping: $F(y)=My+b$ with M positive definite and symmetric, and $Y=\mathbb{R}^m$ (unconstrained). The VI is then fully equivalent to the unconstrained, convex quadratic minimization problem with objective $f(y) = y^tMy + b^ty$. Also, let our algorithm be modified as follows (with the purely rhetorical goal of giving support to the scaling of the BFGS updates).

- First, we keep no cut whatsoever from one iteration to the next, thus being guided only by the single quadratic cut generated each time from the current Jacobian approximation. This implies that the analytic center is the center of the quadratic cut.
- Second, we make no centering steps ever, only an updating step at each iteration; if we did not prohibit them, centering steps could happen, because of the linesearch that is our third and last modification.
- an exact linesearch is performed on each (updating) step, such that f is minimized (the stepsize can be computed analytically).

Then, for this rather special version of the algorithm,

1. the same iteration points are generated as the corresponding quasi-Newton optimization method would generate, and
2. the classical argument [14, pp. 261–262] in favor of spreading the eigenvalues of J_kM^{-1} above and below 1, applies here as well.

We are therefore interested in a scaling of the updates

$$J_{k+1} = J_k + \lambda\left(\frac{F_\Delta F_\Delta^t}{F_\Delta^t y_\Delta} - \frac{J_k y_\Delta y_\Delta^t J_k}{y_\Delta^t J_k y_\Delta}\right), \quad \lambda \in \mathbb{R}^+,$$

that will ensure that the eigenvalues of $J_{k+1}M^{-1}$ include 1 in the interval they span. Let us introduce the notation

$$T_k = M^{-1/2}J_kM^{-1/2}, \quad t_k = M^{1/2}y_\Delta.$$

Then, since $F_\Delta = My_{k+1} + b - My_k - b = My_\Delta$, we have $F_\Delta = M^{1/2}t_k$ and

$$\frac{y_\Delta^t J_k y_\Delta}{y_\Delta^t F_\Delta} = \frac{t_k^t T_k t_k}{t_k^t t_k}.$$

Note also that T_k and J_kM^{-1} are similar, because $M^{1/2}T_kM^{-1/2} = J_kM^{-1}$, and thus have the same eigenvalues $e_1 \leqslant e_2 \leqslant \cdots \leqslant e_m$. Finally, Rayleigh's principle ensures that

$$e_1 \leqslant \frac{t_k^t T_k t_k}{t_k^t t_k} \leqslant e_m$$

so that setting

$$\lambda = \frac{t_k^t t_k}{t_k^t T_k t_k} = \frac{y_\Delta^t F_\Delta}{y_\Delta^t J_k y_\Delta}$$

gives the desired scaling of the eigenvalues.

Note that for the highly specialized problem and algorithm described above, it can be proved that the condition number e_m/e_1 of $J_k M^{-1}$ is no better than that of $J_{k+1}M^{-1}$, so that in theory only a scaling of the initial approximation would be needed. In practice, it is better to use the scaling factor at each iteration.

5. Numerical results

5.1. Notes on the implementation

Here are some details on our implementation of the primal-dual algorithm described above. We used the matrix computation software MATLAB for most computations; the linear programming software CPLEX was used for the gap evaluations.

Sparsity is exploited whenever possible. Within the matrix A, there are columns from the definition of the feasible set Y of the $VI(F, Y)$, usually sparse, and columns from the linear cuts of the algorithm, always dense in our applications. The two categories are treated accordingly. Basically, this means that the matrix A is stored in two parts, $A = [spA \mid \mathrm{d}A]$, respectively sparse and dense, and that a product of type ADA^t where D is a diagonal matrix, is computed as

$$ADA^t = spA \cdot spD \cdot spA^t + \mathrm{d}A \cdot \mathrm{d}D \cdot \mathrm{d}A^t,$$

where spD and $\mathrm{d}D$ are both sparse matrices and denote the parts of D of appropriate dimensions to match spA and dA.

A *linear system* is solved at each update or recentering step, with a Cholesky factorization. Note that sparse techniques cannot be used, as the matrices Δ are dense.

The *positive definiteness* of the Jacobian matrices is important for the quadratic cuts; if, because of round-off error, a (symmetrized) Jacobian ∇_k fails to be positive definite, an over-weighting of the diagonal is used to recover the property. It is performed by adding an identity matrix whose elements are multiplied by $100 \cdot \mathrm{trace}(\nabla) \cdot \mathrm{eps} \cdot 2^{\mathrm{index}}$. Here "eps" is the machine epsilon given by the function of the same name in MATLAB, and "index" is increased one unit at a time, from 1, until positive-definiteness is attained. Note that amongst the problems on which we report below, overweighting was used solely in the two initial iterations of problem `choi.`

The two *linesearches* of the updating step are performed using a Newton method linesearch, with backtracking to remain within the current set Y_k as well as within the quadratic cut.

An *initial center* for the very first iteration is easy to find in many cases with simple sets Y. Otherwise, a feasible point is built ad-hoc and the centering step used to recenter it.

Finally, *backtracking* is used in both the updating and recentering steps, should the full steps lead to a violation of the positivity constraints. The maximum step size that preserves positivity is computed as a simple ratio test over all components that are negative.

5.2. Numerical examples

The primal–dual algorithm was tested on four problems from the variational inequality literature, as well as one lesser-known, but challenging, environmental/economic model for the pricing of pollution permits. The first four problems were described in [1] and in the original papers; only their main characteristics are given along the numerical results, in Section 5.4. The pollution permit pricing model is described in the next Section 5.3. For all the tests below, the results are posted as follows.

In the "Method" column, "primal–dual BFGS" refers to the algorithm described in Sections 2 and 3, the quadratic cuts, being defined with the scaled BFGS approximation of Section 4; "primal–dual Jacobian" indicates the same algorithm, but with Jacobian-based cuts; "Dual Jacobian" refers to the linesearching, dual algorithm put forward in Section 5 of [1]; and "Linear cuts" refers to the plain linear cuts, primal-dual approach of [5] with weighted centers (because of the weighting, one extra evaluation of F is required for each cut). The quadratic cut, dual jacobian algorithm is a reference point for the primal-dual quadratic cut versions. The linear cut algorithm's results highlight the usefulness of the quadratic cuts. The four methods use, respectively and per cut:

Primal–Dual BFGS: one evaluation of F.
Primal–Dual Jacobian: one evaluation of F and one of ∇F.
Dual Jacobian: one evaluation of F and one of ∇F.
Linear cuts: two evaluations of F.

In the "Nb of cuts" and "Centering steps" columns, we report the total number of cuts (and hence updating steps), as well as the number of centering steps. Recall from Section 3 that the dual algorithm takes at least one centering step for each cut.

The "Seconds" column indicates the cpu time, as measured by MATLAB's builtin function. This excludes the initial loading time for the problem `choi`. No cpu times are reported for the example of Section 5.3; time spent on the VI itself is negligible in comparison with the hours required for the computations of the mapping F. All but one problems were run on an Ultra 1/200 Sun workstation with 128M of memory; the MMMR example of Section 5.3 was run on a parallel HP machine of the E.T.H. in Zürich.

The "Gap"column refers to the relative primal gap, see Definition 4, at the approximate center (or weighted center for the linear algorithm), used as stopping criterion. A gap level is used for each problem in relation to the precision desired in the solution.

In almost all cases, the centering level used was 0.9, which performs well most of the time; the only exception are the results for example `choi`, which are given for both centering levels 0.9 and 0.1.

5.3. Pricing of pollution permits: the MMMR model

The markal–macro multi-regional (MMMR) model is a large-scale representation of the energy sectors of many countries, as well as a macro-economic model of their economies. It was developed by a group a researchers at the E.T.H. and the Paul-Scherrer Institute (Zürich); see [15] and the thesis [2]. The model was used for the pricing of CO_2 emission permits: within the context of a pollution permits market, countries are allowed to buy or sell their rights to emit certain amounts of

Table 1
Example MMMR, 10 variables

Method	Nb of cuts	Centering steps	Gap
Primal–dual BFGS	35	56	-1.3×10^{-2}
Linear cuts	75	75	-1.3×10^{-2}

polluting gases. By modeling the impact of pollution restrictions on economic output, the researchers were able to find equilibrium prices in the pollution permits market.

Recall that the trade of pollution permits is one of the pillars of the 1997 Kyoto Protocol.

At the base of the model are national-level submodels of the energy and economic activities of each country, which have typically been developed by independent groups of researchers. The submodels are, in mathematical programming terms, large nonlinear optimization problems. At the international level, these NLPs are linked by an equilibrium problem in the form of a complementarity problem $F(y) \geqslant 0 \;\; y \geqslant 0 \;\; F(y)^t y = 0$, or equivalently a variational problem $VI(F, \mathbb{R}^m_+)$. The function F at point y is the sum of the so-called excess demands obtained by solving each of the national level NLPs, where y is used as a price parameter by the nonlinear programs.

Notice then that:

1. function evaluations are time-consuming: the NLPs considered in [15] each require several minutes of cpu on a mini-supercomputer;
2. the Jacobian ∇F is not defined, let alone easily computable, as the mapping F is known only implicitly.

We report on our results with a three-country, five-time-period, two-product problem described in [15]. The derived VI has ten variables, and the mapping F in question was observed **not** to be monotone, although observations indicate that it appears to be almost pseudo-monotone (meaning that it is pseudo-monotone between most observed pairs of feasible points). Results are as follows, in Table 1.

The MMMR model is challenging because of its undefined Jacobian and its low monotonicity level. Cutting plane methods, in general, are well adapted to such difficult, unstructured, but small-scale problems; but the ACCPM-VI (quadratic cuts) approach with quasi-Jacobian that is put forward in this paper is especially well suited to the problem: keeping quadratic cuts is impossible, given the low monotonicity, but temporary quadratic cuts better that halve the hours-long computing time.

Fig. 4 shows the improvement that can be made by using a scaled BFGS quadratic cut approach, over the weighted-center, linear cut method of [5]. Notice how the quadratic cuts, which technically should apply only to strongly monotone problems, still provide valuable information.

5.4. Results on four problems from the literature

Problem Choi is a mixed complementarity problem (or box-constrained variational inequality) in 13 variables, the problem was described in [20]. We provide results for two levels of gaps (1×10^{-4}

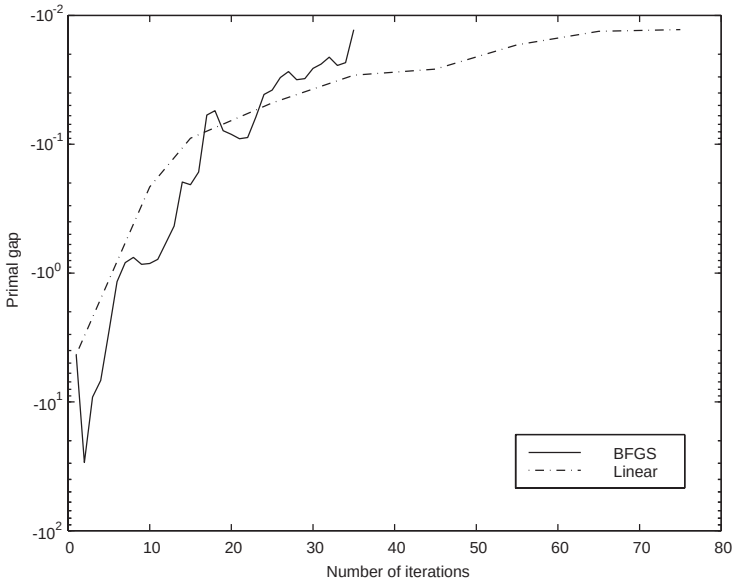

Fig. 4. Example mmmr: gap vs. iterations for two methods.

and 1×10^{-8}), mainly to show that higher precision is easily reachable, although at a cost. Problems Nash10 and qHPHard are respectively 9- and 19-variables problems from the projection-method literature (see [16]); linear and quadratic cuts approaches have fared well against projection methods on these problems, see [1]. Finally, Options is an american option pricing problem, as described in [17,18]. It is interesting to us for its larger size, but it is clear that there are better adapted, linear complementarity algorithm for this problem (see [19] for example). Reported here are the average results for the 24 variational inequalities involved in solving the problem. The results appear in Table 2.

Graphs of the progression of the primal gap with the iterations are provided in Figs. 5 and 6 in the appendix.

In Table 3 we provide our results with the problem choi at a centering criterion of 0.1; results with 0.9 are repeated for ease of comparison.

From this admittedly small sample of problems, one can infer at least two things. First, the primal–dual method and the dual, linesearching method of [1] appear to perform quite similarly: the better centering obtained by the dual method, due to the default centering step incurred at each iteration, seems to compensate the computing overhead of those centering steps. Second, the quasi-Jacobian method solves all the problems from our set, and is usually slightly slower than the Jacobian-based approaches. Of course, it does without the Jacobian, so that this second result is quite attractive for anyone with a VI whose Jacobian is expensive or impossible to compute.

The results seem otherwise quite problem-dependent. One would quickly blame the poor performance of the BFGS in Nash10, on the crudeness of the Jacobian approximation; but how can one explain its behavior in qHPHard, with many fewer cuts required than the primal–dual

Table 2
Numerical results for the four problems

Method	Nb of cuts	Centering steps	Seconds	Gap
Example `Choi`, 13 variables				
Primal–Dual BFGS	12	3	1.91	1×10^{-4}
Primal–Dual Jacbn	10	0	1.58	1×10^{-4}
Dual Jacbn	7	7	1.30	1×10^{-4}
Linear cuts	70	0	11.52	1×10^{-4}
Primal–dual BFGS	35	3	4.41	1×10^{-8}
Primal–dual Jacbn	31	0	3.93	1×10^{-8}
Dual Jacbn	20	20	2.74	1×10^{-8}
Linear cuts	180	0	29.9	1×10^{-8}
Example `Nash10`, 9 variables				
Primal–dual BFGS	20	2	1.25	1×10^{-3}
Primal–dual Jacbn	10	0	0.82	1×10^{-3}
Dual Jacbn	6	6	1.08	1×10^{-3}
Linear cuts	56	0	2.6	1×10^{-3}
Example `qHPHard`, 19 variables				
Primal–dual BFGS	80	0	3.9	1×10^{-3}
Primal–dual Jacbn	91	38	5.0	1×10^{-3}
Dual Jacbn	64	109	4.1	1×10^{-3}
Linear cuts	211	0	8.9	1×10^{-3}
Example `Options`, 100 variables				
Primal–dual BFGS	207	77	43.0	1×10^{-4}
Primal–dual Jacbn	202	77	33.2	1×10^{-4}
Dual Jacbn Linesrch	200	200	37.5	1×10^{-4}
Linear cuts	547	2	52.9	1×10^{-4}

Jacobian, and no centering steps at all ? In this case, the approximate cut gives better results than the exact cut.

6. Conclusion

In this paper, we have introduced a primal–dual algorithm to find the analytic centers used in the ACCPM-VI (quadratic cut) approach of [1]. Primal–dual techniques are robust, and in opposition to dual methods, no supplementary effort is required to obtain a centrality measure. We also present numerical evidence that Jacobian-proxied cuts, based on first-order information, can perform as well as cuts using the Jacobian itself.

The algorithm is successfully used to solve a number of problems from the VI literature, including one very interesting and challenging problem on the pricing of pollution permits.

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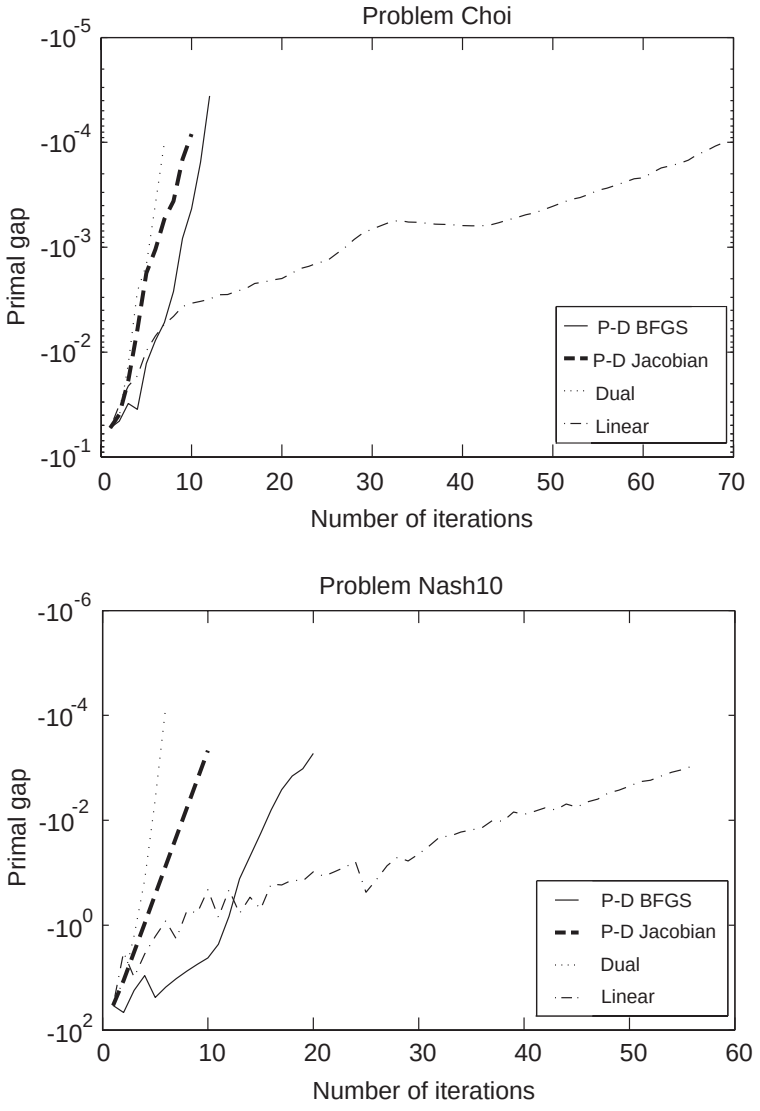

Fig. 5. Progression of gap vs. iterations.

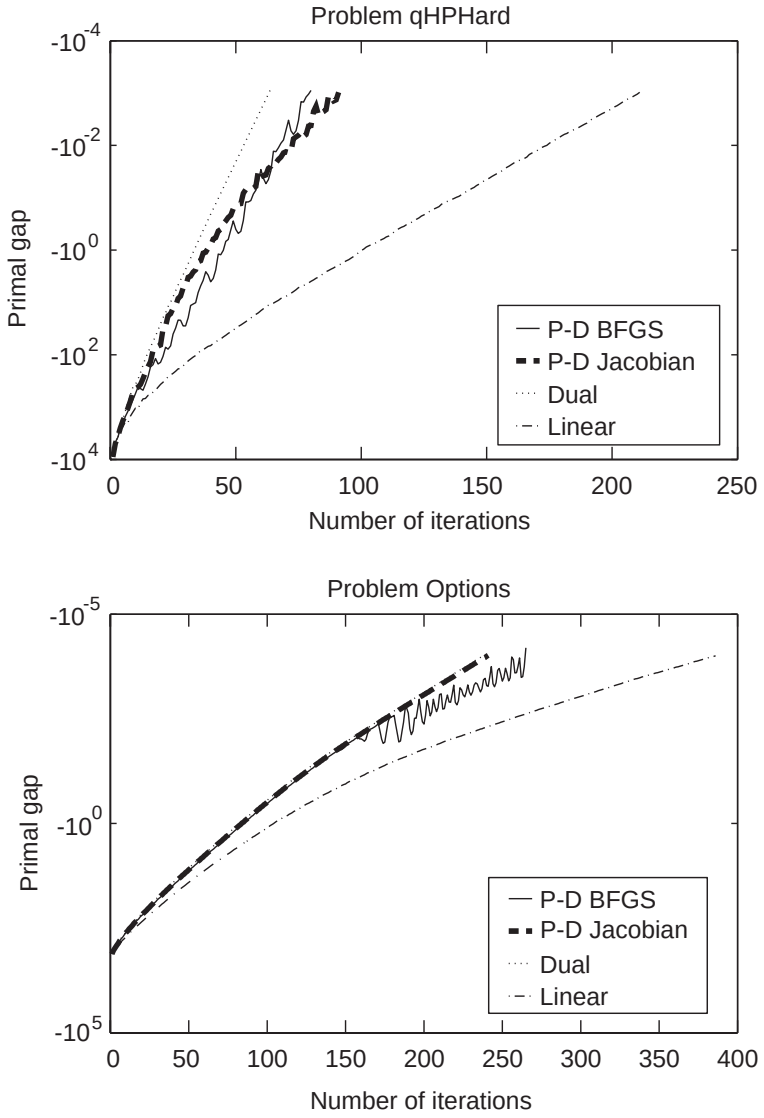

Fig. 6. Progression of gap vs. iterations.

Appendix A.

Graphs of primal gap vs. iterations are given in Figs. 5 and 6.

Table 3
Numerical results for `choi` with more stringent centering

Method	Nb of cuts	Centering steps	Seconds	Gap
Example `Choi`, centered to level 0.9				
Primal–dual BFGS	12	3	1.91	1×10^{-4}
Primal–dual Jacbn	10	0	1.58	1×10^{-4}
Dual Jacbn	7	7	1.30	1×10^{-4}
Linear cuts	70	0	11.52	1×10^{-4}
Example `Choi`, centered to level 0.1				
Primal–dual BFGS	14	14	2.15	1×10^{-4}
Primal–dual Jacbn	8	6	1.40	1×10^{-4}
Dual Jacbn	8	10	1.36	1×10^{-4}
Linear cuts	65	66	11.3	1×10^{-4}

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