Proportionality-Based Gradient Methods with Applications in Contact Mechanics

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Abstract. Two proportionality based gradient methods for the solution of large convex bound constrained quadratic programming problems, MPRGP (Modified Proportioning with Reduced Gradient Projections) and P2GP (Proportionality-based Two-phase Gradient Projection) are presented and applied to the solution of auxiliary problems in the inner loop of an augmented lagrangian algorithm called SMALBE (Semi-monotonic Augmented Lagrangian for Bound and Equality constraints). The SMALBE algorithm is used to generate the Lagrange multipliers for the equality constraints. The performance of the algorithms is tested on the solution of the discretized contact problems by means of TFETI (Total Finite Element Tearing and Interconnecting).

Keywords: QP optimization · Contact problems · P2GP · MPRGP

1 Introduction

This work is focused on the solution of quadratic programming problems characterized by bound constraints and linear equality constraints, i.e. problems of the form

$$\begin{aligned} &\min f(\mathbf{x}) := \tfrac{1}{2}\mathbf{x}^\top \mathsf{A}\,\mathbf{x} - \mathbf{x}^\top \mathbf{b} \\ &\text{s.t.}\ \ \mathsf{B}\mathbf{x} = \mathbf{0} \\ &\qquad \mathbf{x} \in \Omega \end{aligned} \tag{1}$$

where $\mathsf{A} \in \mathbb{R}^{n\times n}$ denotes a symmetric positive definite matrix, $\mathsf{B} \in \mathbb{R}^{m\times n}$ is full rank and $m < n$, so $\operatorname{Ker}\mathsf{B} \neq \{\mathbf{0}\}$, $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$. The set Ω is a closed convex set of the form

$$\Omega = \{\mathbf{x} \in \mathbb{R}^n \ :\ l_i \leq x_i \leq u_i, \quad i = 1, \ldots, n\}.$$

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We admit $l_i = -\infty$ and/or $u_i = \infty$, so that Ω_i can be defined by box or bound constraints.

A number of methods have been proposed for the solution of (1), basically based either on iterior point (see for instance [5,6] and references therein) or active set strategies [15]. In this paper we will just consider algorithms which belong to the latter class. More specifically, we are interested in SMALBE, a variant of Augmented Lagrangian methods which generates approximations for the Lagrange multipliers for the equality constraints in the outer loop and proportionality-based gradient methods for the bound constrained minimization of the lagrangian in the inner loop. A unique feature of SMALBE is a bound on the number of outer iterations which is independent on the conditioning of the constraints. Two algorithms are used for the solution of the auxiliary inner loop problems. The first one is the MPRGP algorithm (Modified Proportioning with Reduced Gradient Projections). A nice feature of MPRGP, which combines conjugate gradient method with gradient projections, is the bound on the rate of convergence in terms of the condition number of the Hessian, so that it can solve a class of problems (1) with the spectrum of A in a given positive interval in a number of iterations which is independent of n [21]. In particular, such property is enjoyed by a class of problems (1) obtained by various discretizations of variational inequalities that describe the equilibrium of a system of bodies in mutual contact, so that the cost of a solution is asymptotically proportional to n (see Dostál et al. [18,20], or [19, Chap. 11]). The second algorithm is P2GP (Proportionality-based Two-phase Gradient Projection), which combines monotonic spectral method with gradient projections and turned out to be very efficient for the solution of several problems [9]. Here we briefly describe the above algorithms and compare their performance on the solution of discretized contact problems of elasticity.

2 The SMALBE Framework

The SMALBE algorithm [12] works with the augmented Lagrangian in the form

$$L(\mathbf{x}, \boldsymbol{\lambda}, \varrho) = \frac{1}{2}\mathbf{x}^\top \mathsf{A}\,\mathbf{x} - \mathbf{x}^\top \mathbf{b} + \mathbf{x}^\top \mathsf{B}^\top \boldsymbol{\lambda} + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}\|^2,$$

where $\boldsymbol{\lambda} \in \mathbb{R}^m$ is the vector of the lagrangian multipliers associated with the linear equality constraints and $\varrho > 0$ is a fixed regularization parameter. In the inner loop, the algorithm carries out an approximate bound constrained minimization of the augmented lagrangian with the precision controlled by a multiple of the feasibility error and the projected gradient

$$g_i^P(\mathbf{x}) \equiv g_i^P(\mathbf{x}, \boldsymbol{\lambda}, \varrho) := \begin{cases} \nabla L_{x_i}(\mathbf{x}, \boldsymbol{\lambda}, \varrho) & \text{if } \ i \in \mathcal{F}(\mathbf{x}), \\ \min\{0, \nabla L_{\mathbf{x}_i}(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\} & \text{if } \ i \in \mathcal{A}_l(\mathbf{x}), \\ \max\{0, \nabla L_{\mathbf{x}_i}(\mathbf{x}, \boldsymbol{\lambda}, \varrho)\} & \text{if } \ i \in \mathcal{A}_u(\mathbf{x}), \end{cases}$$

where

$$\mathcal{F}(\mathbf{x}) = \{i : x_i \in (\ell_i, u_i)\}, \quad \mathcal{A}_\ell(\mathbf{x}) = \{i : x_i = \ell_i\}, \quad \mathcal{A}_u(\mathbf{x}) = \{i : x_i = u_i\}.$$

The minimization in the inner loop can be carried out by any convergent algorithm. Here we use the gradient methods described in the next section. The SMALBE algorithm reads as follows.

Algorithm 1. (SMALBE)

1: $tol \geq 0;\ \ \eta > 0;\ \ 1 > \vartheta > 0;\ \ \varrho > 0;\ \ M_0 = M_1 \in \mathbb{R};\ \ \boldsymbol{\lambda}_0 \in \mathbb{R}^m;\ \ \mathbf{x}^0 \in \mathbb{R}^n;\ \ k = 0;$
2: **while** $(\|\mathbf{g}^P(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho)\| \leq tol$ and $\|\mathsf{B}\mathbf{x}^k\| \leq tol)$ **do** ▷ Main loop
3: Find $\mathbf{x}^{k+1} \in \Omega$ such that
4: $\|\mathbf{g}^P(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^k, \varrho)\| \leq \min\{M_{k+1}\|\mathsf{B}\mathbf{x}^{k+1}\|, \eta\}$ ▷ BQP subproblem
5: $\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \varrho \mathsf{B} x^{k+1}$
6: **if** $(M_{k+1} = M_k$ and $L(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^{k+1}, \varrho) < L(\mathbf{x}^k, \boldsymbol{\lambda}^k, \varrho) + \frac{\varrho}{2}\|\mathsf{B}\mathbf{x}^{k+1}\|)$ **then**
7: $M_{k+2} = \vartheta M_{k+1}$ ▷ Tighten precision control
8: **else**
9: $M_{k+2} = M_{k+1}$
10: **end if**
11: $k = k + 1$
12: **end while**

3 Gradient Methods Based on Proportionality Measures

In the previous section we saw that solving problem (1) by means of the SMALBE framework leads to the solution of a series of quadratic programs subject to bound constraints only (BQPs), i.e. problems of the form

$$\begin{aligned} &\min\ \hat{f}(\mathbf{x}) \\ &\text{s.t.}\ \ l_i \leq x_i \leq u_i, \quad i = 1, \dots, n, \end{aligned}$$

where $\hat{f}(\mathbf{x}) = L(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$.

The minimization of the Lagrangian in Step 4 does not affect $\boldsymbol{\lambda}, \boldsymbol{\varrho}$, so we shall consider in this section cost functions with only one variable.

Many gradient-based methods have been proposed which alternate steps aimed at identifying the variables which are on the bound at the solution (identification) and steps aimed at reducing the objective function on the face determined by the current active set. The latter, in particular, are usually unconstrained minimization steps for the solution of an *auxiliary problem* of the form

$$\begin{aligned} &\min\ \hat{f}(\mathbf{x} + \mathbf{d}) \\ &\text{s.t.}\ \ d_i = 0, \quad i \in \mathcal{A}(\mathbf{x}), \end{aligned} \tag{2}$$

where we have defined the active set as $\mathcal{A}(\mathbf{x}) := \mathcal{A}_\ell(\mathbf{x}) \cup \mathcal{A}_u(\mathbf{x})$. If the minimizer of (2) is unfeasible, a projected line-search is usually used to recover a feasible point on the face under analysis.

A crucial issue in the development of such kind of algorithms is to define suitable criteria to decide how much a face is worth to be explored. Indeed finding an approximate solution for the auxiliary problem with an high level of accuracy may be a computational expensive task, which ends up to be useless if the current active set is far from being the optimal one. To overcome the inefficiencies associated with the use of heuristic criteria such as imposing a maximum number of consecutive minimization steps, some practical termination condition have been proposed in literature. An effective one is the one based on the concept of *proportionality* (see, e.g., Dostál [11], Dostál and Schöberl [21], Friedlander and Martínez [24], or Bielchowsky et al. [3]). An iterate $\mathbf{x}^k$ is called *proportional* if, for a suitable constant $\Gamma > 0$,

$$\|\boldsymbol{\beta}(\mathbf{x}^k)\|^2 \leq \Gamma \widetilde{\boldsymbol{\varphi}}^\top(\boldsymbol{x}^k)\boldsymbol{\varphi}(\mathbf{x}^k), \tag{3}$$

where $\boldsymbol{\varphi}(\mathbf{x})$, $\widetilde{\boldsymbol{\varphi}}^\top(\boldsymbol{x})$, and $\boldsymbol{\beta}(\mathbf{x})$ are the so-called free, reduced free, and chopped gradients, respectively, defined component-wise as

$$\varphi_i := \begin{cases} \nabla L_{\mathbf{x}_i} & \text{if } \ i \in \mathcal{F}, \\ 0 & \text{if } \ i \in \mathcal{A}_l, \\ 0 & \text{if } \ i \in \mathcal{A}_u, \end{cases} \qquad \beta_i := \begin{cases} 0 & \text{if } \ i \in \mathcal{F}, \\ \min\{0, \nabla L_{\mathbf{x}_i}\} & \text{if } \ i \in \mathcal{A}_l, \\ \max\{0, \nabla L_{\mathbf{x}_i}\} & \text{if } \ i \in \mathcal{A}_u, \end{cases}$$

$$\widetilde{\varphi}_i = \begin{cases} \max\{\varphi_i, \frac{u_i - x_i}{\alpha}\} & \text{if } \ \varphi_i < 0, \\ \min\{\varphi_i, \frac{u_i - x_i}{\alpha}\} & \text{if } \ \varphi_i > 0 \end{cases},$$

where for ease of notation the dependence from $\mathbf{x}$ or $(\mathbf{x}, \boldsymbol{\lambda}, \varrho)$ has been omitted. We note that $\mathbf{x}^*$ is stationary for the BQP problem if and only if

$$\|\boldsymbol{\beta}(\mathbf{x}^*)\| + \|\boldsymbol{\varphi}(\mathbf{x}^*)\| = 0,$$

moreover it is easy to show that, for each $\mathbf{x} \in \Omega$, $\boldsymbol{\beta}(\mathbf{x}) + \boldsymbol{\varphi}(\mathbf{x}) = \mathbf{g}^P(\mathbf{x})$. The vector $\boldsymbol{\varphi}$ coincides with the restriction of the gradient to the reduced space (the one containing the current face), therefore it provides a measure of the optimality of the current point with respect to the current face. The vector $\boldsymbol{\beta}$ instead provides a measure of the optimality over the complementarity space. The ratio between the two is in fact the ratio of the norms of the violation of the Karush-Kuhn-Tucker conditions at free and active variables. It has been proved that if the Hessian of the objective function is positive definite, disproportionality of $\mathbf{x}^k$ guarantees that the solution of the BQP problem does not belong to the face determined by the active variables at $\mathbf{x}^k$, and thus exploration of that face is stopped [11]. The idea of proportional iteration has been recently extended to a more general class of linearly constrained problems, i.e. those subject to bound constraints and a single linear constraint [9].

In the following we will briefly introduce two examples of algorithm proposed in literature which can be ascribed to the class of proportionality and gradient-based active-set algorithms, namely the MPRGP [21] and the P2GP [9].

3.1 The MPRGP Algorithm

The MPRGP algorithm is an active set based algorithm which explores the current face by the conjugate gradient method as long as feasible steps are generated and the violation of the KKT conditions on the free set dominates that on the active set, i.e., as long as (3) holds true. If the iteration is not proportional, then the algorithm releases some indices from the active set using the decrease direction $-\boldsymbol{\beta}$, and if the iteration is not feasible, the algorithm proceeds along the conjugate direction as long as possible (feasible halfstep) and then carries out the reduced gradient step with a fixed steplength. Notice that in case of bound constraints, it is possible to take an optimal unconstrained steplength in order to release the active constraints in the direction $-\boldsymbol{\beta}$. The steplength does not change during the computation and its length is based on the analysis of the decrease of the cost function along the gradient path (see, e.g., [14,16,21]).

Algorithm 2. (MPRGP)

$\mathbf{x}^0 \in \Omega$; $tol > 0$; $\alpha \in (0, 2\|\mathsf{A}\|^{-1})$; $\Gamma > 0$; $k = 0$; $\mathbf{g} = \mathsf{A}\mathbf{x}^0 - \mathbf{b}$; $\mathbf{p} = \boldsymbol{\varphi}(\mathbf{x}^0)$
while $(\|\mathbf{g}^P(\mathbf{x}^k)\| > tol)$ **do** ▷ MAIN LOOP
  if $\left(\|\boldsymbol{\beta}(\mathbf{x}^k)\|^2 \le \Gamma\, \widetilde{\boldsymbol{\varphi}}^\top(\boldsymbol{x}^k)\boldsymbol{\varphi}(\mathbf{x}^k)\right)$ **then** ▷ PROPORTIONAL $\mathbf{x}^k$
    $\alpha_{cg} = \mathbf{g}^\top\mathbf{p}/\mathbf{p}^\top\mathsf{A}\mathbf{p}$, $\mathbf{y} = \mathbf{x}^k - \alpha_{cg}\mathbf{p}$ ▷ TRIAL CG STEP
    $\alpha_f = \max\{\alpha \mid \mathbf{x}^k - \alpha\mathbf{p} \in \Omega\}$
    if $(\alpha_{cg} \le \alpha_f)$ **then**
      $\mathbf{x}^{k+1} = \mathbf{y}$; $\mathbf{g} = \mathbf{g} - \alpha_{cg}\mathsf{A}\mathbf{g}$ ▷ CG STEP
      $\beta = \boldsymbol{\varphi}^\top(\mathbf{y})\mathsf{A}\mathbf{p}/\mathbf{p}^\top\mathsf{A}\mathbf{p}$; $\mathbf{p} = \boldsymbol{\varphi}(\mathbf{y}) - \beta\mathbf{p}$
    else ▷ EXPANSION OF ACTIVE SET
      $\mathbf{x}^{k+\frac{1}{2}} = \mathbf{x}^k - \alpha_f\mathbf{p}$; $\mathbf{g} = \mathbf{g} - \alpha_f\mathsf{A}\mathbf{p}$ ▷ FEASIBLE HALFSTEP
      $\mathbf{x}^{k+1} = P_\Omega(\mathbf{x}^{k+\frac{1}{2}} - \alpha\boldsymbol{\varphi}(\mathbf{x}^{k+\frac{1}{2}}))$ ▷ FIXED STEPLENGTH EXPANSION STEP
      $\mathbf{g} = \mathsf{A}\mathbf{x}^{k+1} - \mathbf{b}$; $\mathbf{p} = \boldsymbol{\varphi}(\mathbf{x}^{k+1})$
    end if
  else
    $\mathbf{d} = \boldsymbol{\beta}(\mathbf{x}^k)$; $\alpha_{cg} = \mathbf{g}^\top\mathbf{d}/\mathbf{d}^\top\mathsf{A}\mathbf{d}$ ▷ PROPORTIONING STEP
    $\alpha_{fcg} = \min\{\max\{\alpha \mid \mathbf{x}^k - \alpha\mathbf{d} \in \Omega\}, \alpha_{cg}\}$,
    $\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_{fcg}\mathbf{d}$; $\mathbf{g} = \mathbf{g} - \alpha_{fcg}\mathsf{A}\mathbf{d}$; $\mathbf{p} = \boldsymbol{\varphi}(\mathbf{x}^{k+1})$
  end if
  $k = k + 1$
end while

The expansion is implemented by means of Euclidean projection P_Ω, i.e.,

$$P_\Omega(\mathbf{x}) = \arg\min_{\mathbf{y}\in\Omega} \|\mathbf{y} - \mathbf{x}\|.$$

3.2 The P2GP Algorithm

Gradient projection methods have been widely used for the solution of problems characterized by constraints for which the projection onto the feasible set can be computed cheaply, as in the case of bound constraints. Apart from being easy to implement, gradient projection methods have been shown to have nice identification properties [7], which together with their capability of adding/removing multiple variables to/from the active set in a single iteration, made them a natural choice for the identification of the active constraints in active-set methods. A well-known method based on this approach is the GPCG [25] by Moré and Toraldo, developed for strictly convex quadratic programs subject to bound on the variables. The acronym GPCG stands for "Gradient Projection - Conjugate Gradient", the algorithm indeed alternates between two phases: an identification phase, which performs GP iterations until a suitable face of the feasible set is identified or no reasonable progress toward the solution is achieved, and a minimization phase, which exploits the Conjugate Gradient (CG) method to find an approximate minimizer of the objective function in the reduced space resulting from the previous phase. The global convergence of the GPCG method relies on the global convergence of GP with steplengths satisfying a suitable sufficient decrease conditions [7]. In their recent work, di Serafino et al. [9] developed a new active-set method based on gradient projection, called the P2GP (Proportionality-based Two-phase Gradient Projection). The P2GP can be seen not only as an extension of the original GPCG framework to the solution of a wider class of linearly constrained problems, but also an improvement of the original two-phase algorithm with the introduction of spectral steplengths proposed in literature for gradient methods [8], and the replacement of the original heuristic used for the switch between minimization and identification, with a deterministic rule based on the concept of proportional iterate. This last improvement, from the theoretical point of view, allowed to prove finite termination of the algorithm for strictly convex problems, even in the case of dual degeneracy of the solution. Anyway, apart from the improved theoretical properties, the introduction of the proportionality-based stopping criterion for the termination of the minimization phase, together with the use of Barzilai Borwein-like steplengths [2] of Frassoldati [23] for the gradient projection, which have shown to be effective in several application areas [1,4,10], led to better computational performances with respect to the original GPCG algorithm in the solution of BQPs.

The algorithm for the strictly convex case is sketched in Algorithm 3.

P2GP alternates identification phases, where GP steps satisfying sufficient decrease conditions are performed, and minimization phases, where an approximate solution to the auxiliary problem is searched. Unless a point satisfying the stopping condition is found, the identification phase proceeds either until a promising active set $\mathcal{A}^{k+1}$ is identified (i.e., an active set that remains fixed in two consecutive iterations) or no reasonable progress is made in reducing the objective function, i.e.,

$$\hat{f}^k - \hat{f}^{k+1} \leq \eta \max_{\bar{k} \leq l < k} (\hat{f}^l - \hat{f}^{l+1}), \tag{4}$$

where $\eta \in (0,1)$ is a suitable constant and $\bar{k}$ is the first iteration of the current identification phase. In the minimization phase, an approximate solution to problem (2) is searched for. In detail, the minimization of the auxiliary unconstrained problem is abandoned if an approximation to a stationary point is computed satisfying a criterion similar to (4). The proportionality criterion (3) is used to decide when the minimization phase has to be terminated.

Algorithm 3. (P2GP)

$\mathbf{x}^0 \in \Omega$; $tol \geq 0$; $\eta \in (0,1)$; $\Gamma > 0$; $k = 0$;
$conv = (\|\mathbf{g}^P(\mathbf{x}^k)\| \leq tol)$; $phase1 = .true.$; $phase2 = .true.$
while $(\sim conv)$ **do** ▷ Main loop
  $m = k$;
  while $(phase1)$ **do** ▷ Identification Phase
    $\mathbf{x}^{k+1} = P_\Omega(\mathbf{x}^k - \alpha^k \nabla \hat{f}^k)$ where α^k satisfies suff. decrease conditions [7];
    $conv = (\|\mathbf{g}^P(\mathbf{x}^{k+1})\| \leq tol)$;
    $phase1 = (\mathcal{A}^{k+1} \neq \mathcal{A}^k) \wedge (\hat{f}^k - \hat{f}^{k+1} > \eta \max_{m \leq l < k} (\hat{f}^l - \hat{f}^{l+1})) \wedge (\neg conv)$;
    $k = k + 1$;
  end while
  if $(conv)$ **then**
    $phase2 = .false.$;
  end if
  while $(phase2)$ **do** ▷ Minimization Phase
    Compute an approximate solution $\mathbf{d}^k$ to the auxiliary problem (2);
    $\mathbf{x}^{k+1} = P_\Omega(\mathbf{x}^k + \alpha^k \mathbf{d}^k)$ with α^k such that $\hat{f}^{k+1} \leq \hat{f}^k$;
    $conv = (\|\mathbf{g}^P(\mathbf{x}^{k+1})\| \leq tol)$;
    $phase2 = (\|\boldsymbol{\beta}^{k+1}\| \leq \Gamma \|\boldsymbol{\varphi}^{k+1}\|) \wedge (\neg conv)$;
    $k = k + 1$;
  end while
  $phase1 = .true.$; $phase2 = .true.$;
end while

4 Numerical Results

We have implemented our algorithms in MATLAB and used them to solve stationary 2D contact problems with optional Tresca friction and 3D frictionless contact problems. Let us recall that using the duality, the dicretized contact problem reduces to the problem of finding the minimizer of

$$\begin{aligned} \min\ & \Theta(\boldsymbol{\lambda}) := \tfrac{1}{2}\boldsymbol{\lambda}^\top \mathsf{F} \boldsymbol{\lambda} - \boldsymbol{\lambda}^\top \mathbf{d} \\ \text{s.t.}\ & \mathsf{G}\boldsymbol{\lambda} = \mathbf{0}, \\ & \boldsymbol{\lambda} \in \widetilde{\boldsymbol{\Lambda}}(\boldsymbol{\Psi}), \end{aligned}$$

where $\widetilde{\Lambda}(\boldsymbol{\Psi}) = \Lambda(\boldsymbol{\Psi}) - \widetilde{\boldsymbol{\lambda}}$, with

$$\Lambda(\boldsymbol{\Psi}) = \left\{ (\boldsymbol{\lambda}_n^\top, \boldsymbol{\lambda}_t^\top, \boldsymbol{\lambda}_E^\top,)^\top \;\middle|\; \boldsymbol{\lambda}_n \geq 0,\ \|\boldsymbol{\lambda}_{t,i}\| \leq \Psi_i,\ i = 1, \ldots, n_t \right\}.$$

For 3D frictinless problem and 2D problem with a given (Tresca) friction, the feasible set is defined by bound and/or box inequality constraints as (1) (see, e.g., [17,19]). The same type of problem arises in implementation of any time-step of implicit scheme for transient contact problems [18]. In 3D problems with friction, the box constraints are replaced by separable circular constraints, but the resulting QCQP problem can be solved by similar algorithms. A detailed formulation of contact problems and their effective discretization is out of the scope of this article therefore we refer the reader to and [19] from which we borrowed the notation.

4.1 2D Beam with Material Insets and Coulomb Friction

Our first benchmark is the 2D beam problem depicted in left part of Fig. 1, where inside the "soft" ($E = 4.4\,\text{e+5}$, $\sigma = 0.34$) rectangular beam there are 8 stiff ($E = 1.6\,\text{e+7}$, $\sigma = 0.32$) circular insets. The whole set of bodies is subject to a force applied to the right side of the soft beam as shown in the figure. The discretization of the problem leads to a problem with 2222 variables, 1024 of which are subject either to lower bounds or to both lower and upper bounds, and 60 linear equality constraints. The difficulty of this problem lies in the need for the iterative solver to distribute the global information across several nonlinear interfaces.

We solved six different instances of the problem, characterized by different choices for the boundary forces (F_x, F_y). The results obtained by solving the problem with the SMALBE algorithm equipped either with P2GP or with MPRGP are summarized in Table 1. In particular, the number of variables which are on a bound ($|\mathcal{A}|$), number of outer iterations and Hessian multiplications are shown.

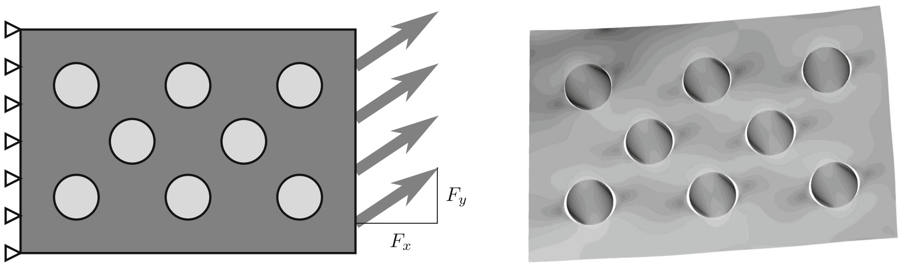


Fig. 1. 2D beam with insets - setting (left) and HMH stress (right)

4.2 Hertz 3D Problem Without Friction

The second benchmark is a 3D two-body contact problem depicted in Fig. 2 (left). The problem was solved by a variant of the FETI method introduced by Farhat and Roux [22] and adapted for contact problems by Dostál et al., see, e.g., [19]. Let us recall that FETI metodology transforms the minimization of convex energy function suject to general inequality and equality constraints in primal formulation to dual problem in Lagramge multipliers for "gluing" of the subdomains and non-penetration. The equality constraints in the dual formulation enable a correct reconstruction of the displacements, while the bound constrainned multipliers for the nonpenetration are related to contact foces (pressure).

The stiff upper body ($E = 1.6\,\text{e+6}$, $\sigma = 0.32$, $\rho = 5.08\,\text{e}{-9}$) is pressed toward the softer lower one ($E = 4.4\,\text{e+5}$, $\sigma = 0.34$, $\rho = 1.04\,\text{e}{-9}$). The upper body has been divided in $3 \times 3 \times 2$ subdomains, while the lower one has been divided in $3 \times 3 \times 3$ subdomains; each subdomain has been divided in $10 \times 10 \times 10$ parts.

Table 1. 2D beam with insets - 6 benchmarks, P2GP × MPGRP comparison

			P2GP				MPRGP			
F_x	F_y	$\|\mathcal{A}\|$	$\|\mathbf{g}^P\|$	$\|\mathsf{Bx}\|$	`out_it`	`Hess`	$\|\mathbf{g}^P\|$	$\|\mathsf{Bx}\|$	`out_it`	`Hess`
100	0	890	1.5e−9	7.0e−7	15	1298	2.7e−14	5.0e−7	19	1667
75	15	879	7.7e−9	1.3e−6	18	1701	5.3e−11	9.9e−7	16	877
75	−15	878	4.0e−9	8.3e−7	16	1427	5.9e−13	8.0e−7	19	1494
−100	0	618	3.8e−9	9.9e−7	14	1432	4.1e−13	5.2e−8	14	1321
−75	15	667	5.8e−9	1.1e−7	16	1625	1.1e−12	1.6e−7	14	1380
−75	−15	666	1.6e−9	6.7e−7	14	1396	2.5e−12	3.9e−7	14	1332

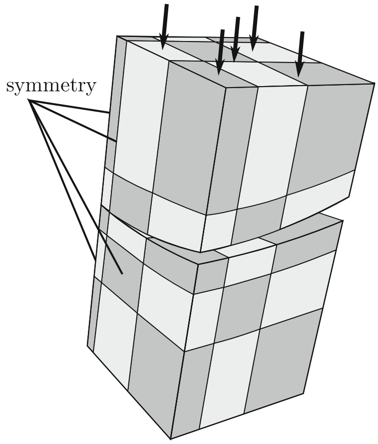
For our test we fixed the radius of the lower body at −50 which translates into a concave surface and we chose two different radii for the upper body, namely 30 and 45. The first problem is characterized by 34854 variables, 900 of them are subject to lower bounds, while the second one is characterized by 34914 variables, 960 of them subject to lower bounds; both problems are subject to 270 linear equality constraints. The problem is not easy as on the solution comprises many dual degenerate components on the boundary of the active contact interface. The performance of both algorithms is summarized in Table 2.

4.3 3D Ball Bearing Without Friction

As last benchmark we chose an example of a real-life application, i.e the 3D multibody contact problem describing the interaction between the various components of a ball bearing; in particular only a segment of the ball bearing is considered (see the right side of Fig. 3). The problem has been solved by means of the same variant of the FETI method used for the previous case. The discretization leads to a QP problem characterized by 19976 variables and 120 linear equality constraints. The active set at the optimal solution consists of 1199 variables among the 1212 subject to a lower bound. In this case the algorithm equipped with P2GP as inner solver took 51 iterations for the solution of the problem, with a total amount of 849 Hessian multiplications, thus outperforming the algorithm equipped with MPRGP which took 60 iterations and a total amount of 1188 Hessian products.

4.4 Comments

The result of the performed tests show that in some cases P2GP appears to be competitive with MPRGP, which is a standard choice for contact problems, and is sometimes able to outperform it. We conjecture that its more aggressive strategy for the expansion the active set performs better in problems where the percentage of active constraints is higher (see for example the case of the ball bearing and the case of the 2D beam). On the other hand, the results in Table 2 indicate that MPRGP is more efficient in treating problems with many dual degenerate components of the solution.



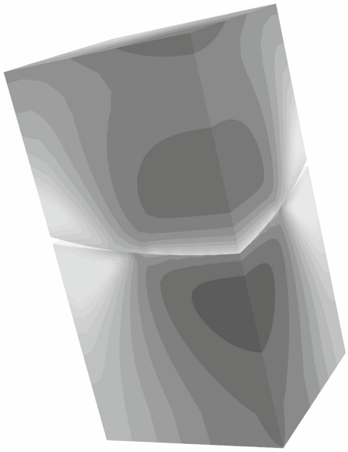
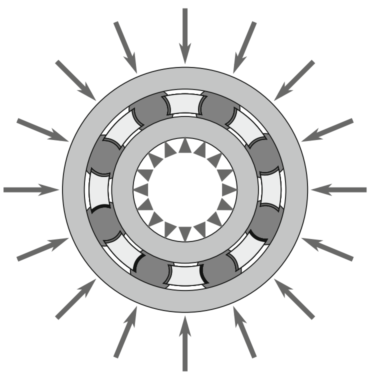


Fig. 2. Herz 3D setting (left) and HMH stress (right)

Table 2. 3D Hertz problem - 2 shape configuration with 4 different pressure for each one - P2GP × MPGRP comparison

r_2	P	$\|\mathcal{A}\|$	P2GP				MPRGP			
			$\|\mathbf{g}^P\|$	$\|\mathsf{B}\mathbf{x}\|$	`out_it`	`Hess`	$\|\mathbf{g}^P\|$	$\|\mathsf{B}\mathbf{x}\|$	`out_it`	`Hess`
30	1	856/900	4.1e−7	3.4e−6	78	1954	4.6e−7	3.6e−6	61	1687
	10	822/900	9.4e−7	3.7e−6	25	2103	8.2e−7	3.6e−6	28	1562
	100	729/900	3.3e−6	3.2e−6	17	2176	3.5e−6	3.3e−6	16	1544
	1000	556/900	1.4e−6	2.2e−6	14	3461	1.3e−6	3.6e−6	12	2447
45	1	887/960	1.5e−7	5.2e−7	34	1900	1.5e−7	5.1e−7	27	1617
	10	821/960	5.1e−7	5.8e−7	20	2306	4.6e−7	6.0e−7	18	1713
	100	659/960	3.3e−7	6.1e−7	13	3301	1.6e−7	5.4e−7	13	2778
	1000	324/960	1.1e−6	9.7e−7	13	3622	9.4e−7	8.5e−7	11	2496



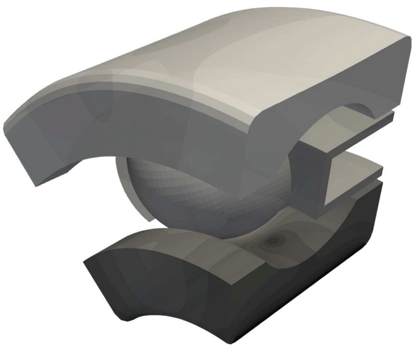


Fig. 3. Ball bearing setting (left) and displacement stress (right)

5 Conclusions

We have presented two methods for the solution of bound or box constrained convex quadratic programming problems. The methods combine monotone spectral gradient method, conjugate gradients, and gradient projections with different steplength choices. The methods were applied to the solution of auxiliary problems in the inner loop of the augmented Lagrangian algorithm for the analysis of 2D and 3D discretized contact problems. The experimental results confirm effectiveness of both algorithms. It seems that a suitable combination of both algorithms can result in still faster solver.

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