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# MINIMIZATION OF A CONVEX QUADRATIC FUNCTION SUBJECT TO SEPARABLE CONICAL CONSTRAINTS IN GRANULAR DYNAMICS

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**Abstract**

The numerical solution of granular dynamics problems with Coulomb friction leads to the problem of minimizing a convex quadratic function with semidefinite Hessian subject to a separable conical constraints. In this paper, we are interested in the numerical solution of this problem. We suggest a modification of an active-set optimal quadratic programming algorithm. The number of projection steps is decreased by using a projected Barzilai-Borwein method. In the numerical experiment, we compare our algorithm with Accelerated Projected Gradient method and Spectral Projected Gradient method on the solution of a particle dynamics problem with hundreds of spherical bodies and static obstacles.

## 1. Time-stepping scheme and formulation of optimization problem

In our simulation, we consider a system of $nb \in \mathbb{N}$ *particles* in vector space $\{(x,y,z) \in \mathbb{R}^3\}$. The position of each particle in time $t$ is defined by the *vector of generalized position* $q_i^{(t)} \in \mathbb{R}^7$, which consists of the position of the centre of gravity $[r_x, r_y, r_z]^T$ and the unit quaternion of rotation $[e_0, e_1, e_2, e_3]^T$. The velocity of the body is defined by the *vector of generalized velocities* $v_i^{(t)} \in \mathbb{R}^6$, it includes the velocity corresponding to the position of the centre of the body and angular velocities represented in Euler angles.

We use the well-known time-stepping scheme, see Heyn [9] or Heyn et al. [10]

$$\begin{aligned} \boldsymbol{q}^{(t+h)} &= \boldsymbol{q}^{(t)} + hQ\boldsymbol{v}^{(t)} , \\ \boldsymbol{v}^{(t+h)} &= \boldsymbol{v}^{(t)} + hM^{-1}(\boldsymbol{F}_{ext} + \boldsymbol{F}_C) , \end{aligned} \tag{1}$$

where $h$ is a time step, $Q$ denotes the matrix of linear mapping between the derivative of the position vector and the vector of velocities, $M$ is a generalized mass matrix, $\boldsymbol{F}_C$ is a vector of forces induced by contact constraints, and $\boldsymbol{F}_{ext}$ is a vector of external forces. In our simulation, the vector of external forces represents the gravity force applied to each body.

Let us denote the number of contacts by $m \in \mathbb{N} \cup \{0\}$. The contact force applied to each body can be separated into the sum of the normal force and the tangential force, i.e.,

$$\boldsymbol{F}_C = \boldsymbol{F}_n + \boldsymbol{F}_T = \gamma_n \boldsymbol{n} + \gamma_u \boldsymbol{u} + \gamma_w \boldsymbol{w} \ ,$$

where $\gamma_n > 0$ is the size of the normal component of the friction force, and $\gamma_u, \gamma_w \in \mathbb{R}$ are the sizes of the tangential components of the friction force. Here, $\{\boldsymbol{n}, \boldsymbol{u}, \boldsymbol{w}\}$ is an orthonormal basis of the tangential space at the contact point. The relation between the components of $\boldsymbol{\gamma}_j := [\gamma_n, \gamma_u, \gamma_w]$ for $j$-th contact ($j = 1, \dots, m$) can be described by the *Coulomb friction model*. The unknown vector of all components in all contacts can be denoted by $\boldsymbol{\gamma} := [\boldsymbol{\gamma}_1, \dots, \boldsymbol{\gamma}_m] \in \mathbb{R}^{3m}$ and can be found by solving the problem of minimizing a convex quadratic function subject to separable conical constraints (see Heyn [9]). The proof of equivalency is based on the maximum dissipation principle and duality.

The optimization problem is given by

$$\text{find} \quad \boldsymbol{\gamma} := \arg\min_{\boldsymbol{x} \in \Omega} f(\boldsymbol{x}), \quad f(\boldsymbol{x}) := \frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x} \ , \tag{2}$$

where $A \in \mathbb{R}^{3m,3m}$ is a symmetric positive semidefinite matrix, $\boldsymbol{b} \in \mathbb{R}^{3m}$, and $\Omega \subset \mathbb{R}^{3m}$ is a non-empty convex feasible set defined by separable conical constraints

$$\Omega := \{\boldsymbol{x} \in \mathbb{R}^{3m} : h_j(x_{2j-2}, x_{2j-1}, x_{2j}) \le 0, j = 1, \dots, m\} \ ,$$

where $h_j : \mathbb{R}^3 \to \mathbb{R}$ are conical constraints functions

$$h_j(x, y, z) := \sqrt{y^2 + z^2} - \mu_j x, \quad j = 1, \dots, m \ ,$$

and $\mu_j \ge 0$ are given friction coefficients that define the interior angles of cones. Let us notice, that if we consider the problem without friction, then $\mu_j = 0$, and the optimization problem (2) becomes a quadratic programming problem with bound constraints.

For the sake of simplicity we denote the triplet of compoments of $\boldsymbol{x} \in \mathbb{R}^n$ constrained by $j$-th constraint function using the notation of index sets

$$\mathcal{I}_j := \{3j-2, 3j-1, 3j\}, \quad \bigcup_{j=1}^{m} \mathcal{I}_j = \{1, \dots, n\}, \quad j = 1, \dots, m \ .$$

## 2. Active-set method

For numerical solution of the problem (2), we are using the variant of Modified Proportioning with Gradient Projection (MPGP), see Dostál [5] and Dostál et al. [7, 4], or Pospíšil [12]. This active-set algorithm is based on the decomposition of the set of all constraint indices $\mathcal{M} := \{1, \dots, m\}$ into two disjoint subsets based on the values of constraint functions

$$\begin{aligned} \mathcal{F}(\boldsymbol{x}) &:= \{j \in \mathcal{M} : h_j(\boldsymbol{x}_{\mathcal{I}_j}) < 0\} \ , \\ \mathcal{A}(\boldsymbol{x}) &:= \{j \in \mathcal{M} : h_j(\boldsymbol{x}_{\mathcal{I}_j}) = 0\} \ . \end{aligned}$$

The gradient of the objective function $\boldsymbol{g} := \nabla f(\boldsymbol{x}) = A\boldsymbol{x} - b \in \mathbb{R}^n$ can be used to define the *free* and the *chopped* gradient with components

$$\begin{array}{ll} \boldsymbol{\varphi}_{\mathcal{I}_j}(\boldsymbol{x}) = \boldsymbol{g}_{\mathcal{I}_j} \text{ for } j \in \mathcal{F}(\boldsymbol{x}), & \boldsymbol{\varphi}_{\mathcal{I}_j}(\boldsymbol{x}) = 0 \text{ for } j \in \mathcal{A}(\boldsymbol{x}), \\ \boldsymbol{\beta}_{\mathcal{I}_j}(\boldsymbol{x}) = 0 \text{ for } j \in \mathcal{F}(\boldsymbol{x}), & \boldsymbol{\beta}_{\mathcal{I}_j}(\boldsymbol{x}) = \boldsymbol{g}_{\mathcal{I}_j} - \min\{n_j^T(\boldsymbol{x}_{\mathcal{I}_j})\boldsymbol{g}_{\mathcal{I}_j}, 0\} n_j(\boldsymbol{x}_{\mathcal{I}_j}) \\ & \hfill \text{for } j \in \mathcal{A}(\boldsymbol{x}), \end{array}$$

where $n_j(x,y,z)$ is the unit outer normal of $j$-th constraint $h_j(x,y,z)$. We consider a problem with conical constraints, so outer normal is given by

$$n_j(x,y,z) := \begin{cases} [-1,0,0]^T & \text{if } x = y = z = 0 \ , \\ \left[-\mu_j, y/\sqrt{y^2+z^2}, z/\sqrt{y^2+z^2}\right]^T & \text{elsewhere.} \end{cases}$$

Algorithm 1: **Modified Proportioning with Barzilai-Borwein Gradient Projection (MPGPS-BB).**

*Choose* $\boldsymbol{x}^0 \in \Omega$
**for** $k = 0, 1, 2, \ldots$ *(while a stopping criterion is not achieved)*
  **if** $\|\varphi(x_k)\| \geq \|\beta(x_k)\|$ (proportioning condition)
    Control the solvability
      **if** $\min\{\alpha_f, \alpha_{cg}\} = \infty$, *then the problem has no solution.*
    CG step *or* CG halfstep
      *make one CG step to solve problem on free set*
      *if this step means leaving* $\Omega$*, do only a half-step and restart CG*
  **else**
    Gradient projection step.
      *make projected Barzilai-Borwein step*
      *restart CG on free set*
  **endif**
  $k := k + 1$
**endfor**

Our algorithm is based on using the free and chopped gradient to minimize the objective function on the free set and afterwards on the active set. The switching between these processes is realized by the proportioning condition. The implementation details of each step are the same as in the original Modified Proportioning with Gradient Projections algorithm (MPGP) in Dostál [5], Dostál et al. [7, 4]. Nevertheless, MPGP was developed to solve the problems with a symmetric positive definite Hessian matrix. The recent generalization to the problems with symmetric positive semidefinite Hessian suggests only one difference from the original algorithm, specifically a test of the problem solvability, see Algorithm 1. The coefficient $\alpha_f$ is the maximal feasible step-size and $\alpha_{cg}$ is a coefficient of the conjugate gradient computed from the free gradient. If both of these coefficient are equal to infinity, then the problem has no solution. The theory will be published in [6].

To solve a problem with separable conical constraints, we suggest to use the projected version of Barzilai-Borwein method [2] instead of the projected gradient method with constant step-length as in original MPGP algorithm. Constant step-length always induces the descend of cost function, as it was shown by Dostál and Schöberl [8]. However, the numerical experiments show that using non-monotone algorithms, such as projected Barzilai-Borwein (PBB) given by

$$\boldsymbol{x}^{k+1} = P_\Omega(\boldsymbol{x}^k - \alpha_k^{BB} \nabla f(x^k)), \quad \alpha_k^{BB} = \frac{\boldsymbol{s}_k^T \boldsymbol{s}_k}{\boldsymbol{s}_k^T A \boldsymbol{s}_k}, \quad \boldsymbol{s}_k = \boldsymbol{x}^k - \boldsymbol{x}^{k-1},$$

usually evokes the decrease of the projection steps number. This modification was inspirated by the Spectral Projected Gradient method (SPG), which uses the similar type of steps, see Birgin et al. [3]. The idea of the combination of MPGP and PBB was firstly presented by Pospíšil [12] and tested on the problem with separable quadratic constraints.

The main shortage of the presented MPGPS-BB algorithm is the absence of the proof of convergence. The PBB method is non-monotone and hardly analyzable. Therefore, the SPG method is using an additional line-search method to control the descend of the objective function, i.e. the global convergence. In our algorithm, we tried to omit this line-search. Our idea is well-founded by the numerical experiment presented in the final section of this paper.

As a stopping criterion in our algorithm, we are using the norm of the *scaled projected gradient* defined by

$$\tilde{\boldsymbol{g}}_\alpha^P(\boldsymbol{x}) := \frac{1}{\alpha}(\boldsymbol{x} - P_\Omega(\boldsymbol{x} - \alpha \nabla f(\boldsymbol{x}))) \ .$$

The equivalency of this gradient and the fulfilment of Karush-Kuhn-Tucker optimality conditions for problems with feasible sets with strong curvature was discussed and proved by Bouchala et al. [4].

## 3. Numerical experiments

In this section, we present the numerical results showing the efficiency of our algorithm on the simulation of 339 spherical particles with friction. In our benchmark, the particles are scattered into simple box represented by six walls. The initial position of the partices and final position can be found in Fig. 1, where we depicted only the partices and the bottom side of the static box. The material of the bodies is represented by density $\rho = 730$ kg.m$^{-3}$ and friction parameter $\mu = 0.3$. The stepsize of the time-stepping scheme is $h = 6.25 \cdot 10^{-4}$ s.

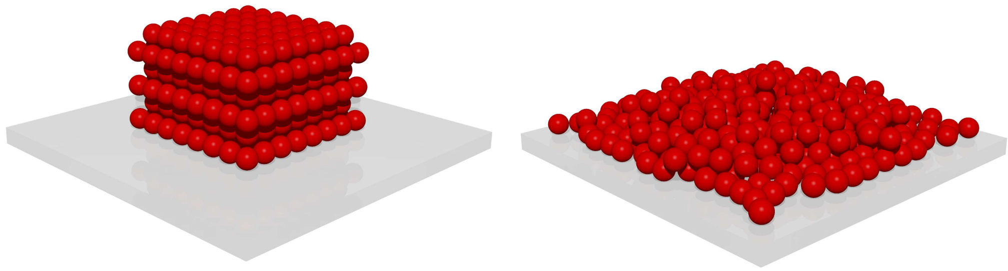

Figure 1: State of testing benchmark at $t = 0$s (left) and $t = 5$s (right).

| t | contacts | n | active | MPGPS-BB | SPG | APGD |
|---|---|---|---|---|---|---|
| 1s | 738 | 2214 | 562 (76%) | 274 (7.6s) | 2360 (37.8s) | 754 (9.4s) |
| 2s | 702 | 2106 | 574 (82%) | 137 (3.4s) | 449 (6.0s) | 346 (2.9s) |
| 3s | 730 | 2190 | 558 (76%) | 137 (3.7s) | 449 (6.0s) | 346 (4.1s) |
| 4s | 814 | 2442 | 640 (79%) | 338 (9.9s) | 2931 (56.2s) | 1345 (18.9s) |
| 5s | 818 | 2454 | 652 (80%) | 425 (12.3s) | 4176 (88.0s) | 1742 (25.6s) |

Table 1: The optimization problems at selected times of the simulation; number of contacts, dimension of the problem, the number of iterations and computing time of the algorithms.

We compare our algorithm with SPG and the Accelerated Projected Gradient Descend method (APGD [11]). In SPG, because the minimum of the quadratic function in a given direction is known, we use the Cauchy step-size instead of using an additional Grippo-Lampariello-Lucidi line-search. All algorithms were implemented in the Matlab environment. For contact detection, we are using our own implementation of the *Moving Bounding-Box algorithm* [13]. The number of iterations at selected times of the simulation can be found in Table 1. We demand the relative stopping tolerance $\|\tilde{\boldsymbol{g}}^P_\alpha(\boldsymbol{x})\| < \epsilon\|b\|, \epsilon = 10^{-6}$.

## 4. Conclusions

In our paper, we proposed the modification of our active-set algorithm for the solution of optimization problem in particle dynamics with friction. Our numerical experiment shows the efficiency of the modifications. Unfortunately, the basic disadvantage of using the projected Barzilai-Borwein method is the absence of a convergence proof as well as of an estimate of the speed of convergence.


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