

Lecture 3. Solvers for the time-discretized problems.

Vincent Acary

Outline

The Quadratic Programming (QP) problem

The Non Linear Programming (NLP) problem

The linear complementarity problem (LCP)

More general complementarity problems

The Variational Inequalities (VI) and the Quasi-Variational Inequalities (QVI)

Nonsmooth and Generalized equations.

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# Quadratic Programming (QP) problem

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## Definition (Quadratic Programming (QP) problem)

Let  $Q \in \mathbb{R}^{n \times n}$  be a symmetric matrix. Given the matrices  $A \in \mathbb{R}^{m_i \times n}$ ,  $C \in \mathbb{R}^{m_e \times n}$  and the vectors  $p \in \mathbb{R}^n$ ,  $b \in \mathbb{R}^{m_i}$ ,  $d \in \mathbb{R}^{m_e}$ , the Quadratic Programming (QP) problem is to find a vector  $z \in \mathbb{R}^n$  denoted by  $\text{QP}(Q, p, A, b, C, d)$  such that

$$\begin{aligned} \text{minimize} \quad & q(z) = \frac{1}{2} z^T Q z + p^T z \\ \text{subject to} \quad & A z - b \geq 0 \\ & C z - d = 0 \end{aligned} \tag{1}$$

## Associated Lagrangian function

With this constrained optimization problem, a Lagrangian function is usually associated

$$\mathcal{L}(z, \lambda, \mu) = \frac{1}{2} z^T Q z + p^T z - \lambda^T (A z - b) - \mu^T (C z - d) \tag{2}$$

where  $(\lambda, \mu) \in \mathbb{R}^{m_i} \times \mathbb{R}^{m_e}$  are the Lagrange multipliers.

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## First order optimality conditions

The first order optimality conditions or Karush-Kuhn-Tucker (KKT) conditions of the QP problem(1) with a set of equality constraints lead to the following MLCP :

$$\begin{cases} \nabla_z \mathcal{L}(\bar{z}, \lambda, \mu) = Q\bar{z} + p - A^T \lambda - C^T \mu = 0 \\ C\bar{z} - d = 0 \\ 0 \leq \lambda \perp A\bar{z} - b \geq 0 \end{cases} . \quad (3)$$

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## Basic properties

- The matrix  $Q$  is usually assumed to be a symmetric positive definite (PD).  
→ the QP is then convex and the existence and the uniqueness of the minimum is ensured providing that the feasible set  $C = \{z, Az - b \geq 0, Cz - d = 0\}$  is none empty.
- Degenerate case.
  - $Q$  is only Semi-Definite Positive (SDP) matrix. (Non existence problems).
  - $A$  (or  $C$ ) is not full-rank. The constraints are not linearly independent. (Non uniqueness of the Lagrange Multipliers)
  - The strict complementarity does not hold. (we can have  $0 = \bar{z} = \lambda = 0$  at the optimal point. )

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## The dual problem and the Lagrangian relaxation

Due to the particular form of the Lagrangian function, the QP problem is equivalent to solving

$$\min_z \max_{\lambda \geq 0, \mu} \mathcal{L}(z, \lambda, \mu) \quad (4)$$

The idea of the Lagrangian relaxation is to invert the min and the max introducing the dual function

$$\theta(\lambda, \mu) = \min_z \mathcal{L}(z, \lambda, \mu) \quad (5)$$

and the dual problem

$$\max_{\lambda \geq 0, \mu} \theta(\lambda, \mu) \quad (6)$$

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## The dual problem and the Lagrangian relaxation

In the particular case of a QP where the matrix  $Q$  is non singular, the dual function is equal to :

$$\begin{aligned}\theta(\lambda, \mu) &= \min_z \mathcal{L}(z, \lambda, \mu) = \mathcal{L}(Q^{-1}(A^T \lambda + C^T \mu - p), \lambda, \mu) & (7) \\ &= -\frac{1}{2}(A^T \lambda + C^T \mu - p)^T Q^{-1}(A^T \lambda + C^T \mu - p) + b^T \lambda + d^T \mu & (8)\end{aligned}$$

and we obtain the following dual problem

$$\max_{\lambda \geq 0, \mu} -\frac{1}{2}(A^T \lambda + C^T \mu - p)^T Q^{-1}(A^T \lambda + C^T \mu - p) + b^T \lambda + d^T \mu \quad (9)$$

which is a QP with only inequality constraints of positivity.

## Equivalences.

The strong duality theorem asserts that if the matrices  $Q$  and  $AQ^{-1}A^T$  are symmetric semi-definite positive, then if the primal problem (1) has an optimal solution then the dual has also an optimal solution.

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## Algorithms for QP

For the standard case

- Active sets methods. see Fletcher book's FLETCHER (1987)
- Interior point methods. see BONNANS *et al.* (2003)
- Projection and splitting methods for large scale problems.

For the degenerate case,

- Lagrangian relaxation
- Active sets methods. see FLETCHER (1993).
- Proximal point algorithm

## Interest of the QP problem

- Reliability with SDP matrix
- Minimization algorithms imply stability



## Definition (Nonlinear Programming (NLP) Problem)

Given a differentiable function  $\theta : \mathbb{R}^n \mapsto \mathbb{R}$ , and two differentiable mappings  $g : \mathbb{R}^n \mapsto \mathbb{R}^{m_i}$   $g : \mathbb{R}^n \mapsto \mathbb{R}^{m_e}$ , the Nonlinear Programming (NLP) problem is to find a vector  $z \in \mathbb{R}^n$  such that

$$\begin{aligned} & \text{minimize} && f(z) \\ & \text{subject to} && g(z) \geq 0 \\ & && h(z) = 0 \end{aligned} \tag{10}$$

## Associated Lagrangian function

The Lagrangian of this NLP problem is introduced as follows

$$\mathcal{L}(z, \lambda, \mu) = f(z) - \lambda^T g(z) - \mu^T h(z) \tag{11}$$

where  $(\lambda, \mu) \in \mathbb{R}^{m_i} \times \mathbb{R}^{m_e}$  are the Lagrange multipliers.

## First order optimality conditions

The Karush-Kuhn-Tucker (KKT) necessary conditions for the NLP problem are given the following NCP:

$$\begin{cases} \nabla_z \mathcal{L}(z, \lambda, \mu) = \nabla_z f(z) - \nabla_z^T g(z) \lambda - \nabla_z^T h(z) \mu = 0 \\ h(z) = 0 \\ 0 \leq \lambda \perp g(z) \geq 0 \end{cases} \quad (12)$$

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## Definition (Linear Complementarity Problem (LCP))

Given  $M \in \mathbb{R}^{n \times n}$  and  $q \in \mathbb{R}^n$ , the Linear Complementarity Problem, is to find a vector  $z \in \mathbb{R}^n$ , denoted by  $LCP(M, q)$  such that

$$0 \leq z \perp Mz + q \geq 0 \quad (13)$$

The inequalities have to be understood component-wise and the relation  $x \perp y$  means  $x^T y = 0$ .

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## Basic properties

- The  $LCP(M, q)$  is that it admits a unique solution for all  $q \in \mathbb{R}^n$  if and only if  $M$  is a P-matrix.  
A P-Matrix is a matrix with all of its principal minors positive, see (COTTLE *et al.*, 1992 ; MURTY, 1988).
- In the worst case, the problem is N-P hard .i.e. there is no polynomial-time algorithm to solve it.
- In practice, this "P-matrix" assumption is difficult to ensure via numerical computation, but a definite positive matrix (not necessarily symmetric), which is a P-matrix is often encountered.

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## Definition (Mixed Linear Complementarity Problem (MLCP))

Given the matrices  $A \in \mathbb{R}^{n \times n}$ ,  $B \in \mathbb{R}^{m \times m}$ ,  $C \in \mathbb{R}^{n \times m}$ ,  $D \in \mathbb{R}^{m \times n}$ , and the vectors  $a \in \mathbb{R}^n$ ,  $b \in \mathbb{R}^m$ , the Mixed Linear Complementarity Problem denoted by  $\text{MLCP}(A, B, C, D, a, b)$  consists in finding two vectors  $u \in \mathbb{R}^n$  and  $v \in \mathbb{R}^m$  such that

$$\begin{cases} Au + Cv + a = 0 \\ 0 \leq v \perp Du + bv + b \geq 0 \end{cases} \quad (14)$$

## Comments

The MLCP is a mixture between a LCP and a system of linear equations. Clearly, if the matrix  $A$  is non singular, we may solve the embedded linear system to obtain  $u$  and then reduced the MCLP to a LCP with  $q = b - DA^{-1}a$ ,  $M = b - DA^{-1}C$ .

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## Link with the QP

If the matrix  $M$  of  $\text{LCP}(M, q)$  is symmetric PD, a QP formulation of (13) is direct into  $\text{QP}(M, q, I_{n \times n}, 0_n, \emptyset, \emptyset)$ ,  $m_i = n$ ,  $m_e = 0$ . For a non symmetric PD matrix  $M$ , the inner product may be chosen as an objective function:

$$\begin{aligned} & \text{minimize} && q(z) = z^T(q + Mz) \\ & \text{subject to} && q + Mz \geq 0 \\ & && z \geq 0 \end{aligned} \quad (15)$$

and to identify (15) with (1), we set

$Q = M + M^T$ ,  $Az = (Mz, z)^T$ ,  $b = (-q, 0)^T$ ,  $m_i = 2n$ ,  $m_e = 0$ . Moreover, the first order optimality condition may be written as

$$\begin{cases} (M + M^T)\bar{z} + p - A^T\lambda - M^T\mu \geq 0 \\ z^T((M + M^T)\bar{z} + p - A^T\lambda - M^T\mu) = 0 \\ \mu \geq 0 \\ u^T(q + M\bar{z}) = 0 \end{cases} \quad (16)$$

Let us recall that a non symmetric matrix  $M$  is PD if and only if its symmetric part,  $(M + M^T)$  is PD.

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## Algorithms for LCP

- Splitting based methods
- Generalized Newton methods
- Interior point method
- Pivoting based method
- QP methods for a SDP matrix.

## Definition (Complementarity Problem (CP))

Given a cone  $K \subset \mathbb{R}^n$  and a mapping  $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ , the Complementarity Problem is to find a vector  $x \in \mathbb{R}^n$  denoted by  $\text{CP}(K, F)$  such that

$$K \ni x \perp F(x) \in K^* \quad (17)$$

where  $K^*$  is the dual (negative polar) cone of  $K$  defined by

$$K^* = \{d \in \mathbb{R}^n, v^T d \geq 0, \forall v \in K\} \quad (18)$$



## Definition (Nonlinear Complementarity Problem (NCP))

Given a mapping  $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ , find a vector  $z \in \mathbb{R}^n$  denoted by NCP( $F$ ) such that

$$0 \leq z \perp F(z) \geq 0 \quad (19)$$

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## Definition (Mixed Nonlinear Complementarity Problem (MiCP))

Given two mappings  $F : \mathbb{R}^{n_1} \times \mathbb{R}_+^{n_2} \mapsto \mathbb{R}^{n_1}$  and  $H : \mathbb{R}^{n_1} \times \mathbb{R}_+^{n_2} \mapsto \mathbb{R}^{n_2}$ . The MiCP is to find a pair of a vectors  $u, v \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$  such that

$$\begin{cases} G(u, v) = 0 \\ 0 \leq v \perp H(u, v) \geq 0 \end{cases} \quad (20)$$

The following definition is equivalent:

## Definition (Mixed Complementarity Problem (MiCP))

Given two sets of indexes  $C$  (for constrained) and  $F$  (for free) forming a partition of the set  $\{1, 2, \dots, n\}$  and two mappings  $F_C : \mathbb{R}^n \mapsto \mathbb{R}^c$ ,  $F_F : \mathbb{R}^n \mapsto \mathbb{R}^f$ , such that  $f + c = n$ , find a vector  $z \in \mathbb{R}^n$  such that

$$\begin{cases} F_F(z) = 0, z_F \text{ free} \\ 0 \leq z_C \perp F_C(z) \geq 0 \end{cases} \quad (21)$$

## Algorithms for Complementarity problems (CP)

- General Complementarity problems. (unstructures  $K$ )
  - General algorithms for VI/CP. (see after)
  - Slow and inefficient algorithm.
- CP on polyhedral cone. (NLP, MiCP)
  - Josephy-Newton method. Linearizing procedure of  $F$ . Newton scheme. Successive LCP resolution.
  - Reformulation into a non equations. Use of generalized Newton method.

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## Definition (Variational Inequality (VI) problem)

Let  $X$  be a nonempty subset of  $\mathbb{R}^n$  and let  $F$  be a mapping from  $\mathbb{R}^n$  into itself. The Variational Inequality problem, denoted by  $VI(X, F)$  is to find a vector  $z \in \mathbb{R}^n$  such that

$$F(z)^T(y - z) \geq 0, \forall y \in X \quad (22)$$

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## Basic properties

- the set  $X$  is assumed to be closed and convex. In most of the applications,  $X$  is polyhedral. The function is also assumed to be continuous, nevertheless some VI are defined for set-valued mappings.
- If  $X$  is a closed set and  $F$  continuous, the solution set of  $\text{VI}(X, F)$  denoted by  $\text{SOL}(X, F)$  is always a closed set.
- A geometrical interpretation of the  $\text{VI}(X, F)$  leads to the equivalent formulation in terms of inclusion into a normal cone of  $X$ , i.e.,

$$-F(x) \in N_{Xx} \quad (23)$$

or equivalently

$$0 \in F(x) + N_{Xx} \quad (24)$$

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## Basic properties

- It is noteworthy that the  $VI(X, F)$  extends the problem of solving non linear equations,  $F(x) = 0$  taking  $X = \mathbb{R}^n$ .
- If  $F$  is affine function,  $F(x) = Mx + q$ , the  $VI(X, F)$  is called Affine VI denoted by,  $AVI(X, F)$ .
- If  $X$  is polyhedral, we say that the  $VI(X, F)$  is linearly constrained, or that is a linearly constrained VI. A important case is the box constrained VI where the set  $X$  is a closed rectangle (possibly unbounded) of  $\mathbb{R}^n$ , i.e

$$K = \{x \in \mathbb{R}^n, -\infty \leq a_i \leq x \leq b_i \leq +\infty\} \quad (25)$$

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## Algorithms for VI

- General VI (unstructured closed convex set  $K$ ).  
Reformulation with the normal map associated the  $VI(K, F)$

$$\mathbf{F}_K^{nor}(z) = F(\Pi_K(z)) + z - \Pi_K(z) \quad (26)$$

A solution  $x$  of the  $VI(K, F)$  is given by  $\mathbf{F}_K^{nor}(z) = 0$  with  $x = \Pi_K(z)$

- General projection algorithm for VI/CP. (Fixed point). Need at least the definition of the projection onto the cone.  
→ Slow and inefficient algorithm.
- Newton Methods for VI/CP. Need the definition of the projection and the Jacobian of  $\mathbf{F}_K^{nor}(z)$   
→ Difficult computation for a unstructured closed convex set  $K$
- If the problem has a better structure, the problem is then reformulated into a specific complementarity problem through a nonsmooth equation.

## Definition (Generalized Equation (GE) problem)

Let  $\Omega \subset \mathbb{R}^n$  be an open set. Given a continuously Fréchet differentiable mapping  $F : \Omega \subset \mathbb{R}^n \mapsto \mathbb{R}^n$  and a maximal monotone operator  $T : \mathbb{R}^n \rightsquigarrow \mathbb{R}^n$ , find a vector  $z \in \mathbb{R}^n$  such that

$$0 \in F(z) + T(z) \quad (27)$$



## Basic properties

The GE problem is closely related to CP problems and to the NLP. For instance, the NCP (19) can be represented into a GE by

$$0 \in F(z) + N_{\mathbb{R}_+^n}(z) \quad (28)$$

and the MCP (12), which provides the KKT necessary conditions for the NLP can be casted into a GE of the form

$$0 \in F(z) + N_K(z), z \in \mathbb{R}^{n+m_e+m_i} \quad (29)$$

with

$$\begin{cases} F(z) = \begin{bmatrix} \nabla \mathcal{L}(z, u, v) \\ -g(z) \\ -h(z) \end{bmatrix} \\ K = \mathbb{R}^n \times \mathbb{R}_+^{m_i} \times \mathbb{R}^{m_e} \end{cases} \quad (30)$$

## Key idea

Reformulation of the Generalized equation into a non smooth equation with good properties (semi-smoothness)

$$0 \in F(z) + T(z) \Rightarrow \Phi(z) = 0 \quad (31)$$

Apply Generalized Newton Method to the equation  $\Phi(z) = 0$ .

## Generalized Newton Method

Solve the equation

$$\Phi(z) = 0 \quad (32)$$

by the extended linearizing procedure.

$$z_{k+1} = z_k - H_k^{-1}(x_k)\Phi(x_k) \quad (33)$$

where  $H_k(x_k)$  is an element of the subdifferential  $\partial\Phi(x_k)$ .

## Definition

**NCP functions.** A function  $\psi : \mathbb{R}^2 \rightarrow \mathbb{R}$  is called a NCP function if it satisfies the following relation

$$\psi(w, z) = 0 \Leftrightarrow 0 \leq w \perp z \geq 0 \quad (34)$$

## Example

$$\psi_{\min}(w, z) = \min(w, z) \quad (35)$$

$$\psi_{FB}(w, z) = \sqrt{z^2 + w^2} - z - w \text{ (Fischer-Burmeister function)} \quad (36)$$

$$\psi_{FB1}(w, z) = \lambda(\psi_{FB}) - (1 - \lambda) \max(0, z) \max(0, w) \text{ with } \lambda \in ]0, 1[ \quad (37)$$

$$\psi_{\text{smooth}}(w, z) = wz + \frac{1}{2} \min^2(0, z + w) \quad (38)$$

## Basic properties

- If the NCP function is everywhere differentiable, the Jacobian is singular at the solution point
- The NCP function needs to be semi-smooth to obtain convergence results.
- Line search methods based on a merit function. For instance,

$$\Psi = \frac{1}{2} \Phi^T(z) \Phi(z) \quad (39)$$

For Fischer-Burmeister function, this function is differentiable everywhere.

→ Stability (global convergence) and local quadratic convergence results.

# Summary of the time-discretized equations

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The discretization of the equation of motion and of the contact law can be summarized in the following system :

$$(\mathcal{P}_{LR}) \quad \begin{cases} U_{k+1} = WP_{k+1} + V_{free} \\ \text{NonSmoothLaw}[U_{k+1}, P_{k+1}] \end{cases} \quad (\text{Unilateral contact, friction and})$$

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$$(\mathcal{P}_{LM}) \quad \left\{ \begin{array}{ll} \mathbb{M}v_{k+1} + \hat{f} = p_{k+1} + G^T \mu_{k+1} & \\ \widehat{G} v_{k+1} = 0 & \text{(Bilateral Constraints)} \\ U_{k+1} = H^T v_{k+1}, p_{k+1} = HP_{k+1} & \text{(Kinematics Relations)} \\ \text{NonSmoothLaw}[U_{k+1}, P_{k+1}] & \text{(Unilateral contact, friction)} \end{array} \right.$$

where

$$\hat{f} = \mathbb{M}v_k + [-hCv_k - hKq_k - h^2\theta Kv_k + h[\theta(F_{\text{ext}})_{k+1}] + (1-\theta)(F_{\text{ext}})_k]$$

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$$(\mathcal{P}) \quad \left\{ \begin{array}{ll} F(v_{k+1}) = p_{k+1} & \text{(Non linear Discret)} \\ G(v_{k+1}) = 0 & \text{(Bilateral Constrai)} \\ U_{k+1} = H^*(q_{k+1})v_{k+1}, r_{k+1} = H(q_{k+1})P_{k+1} & \text{(Kinematics Relati)} \\ \text{NonSmoothLaw}[U_{k+1}, P_{k+1}] & \text{(Unilateral contact)} \end{array} \right.$$

Let us consider the problem  $(\mathcal{P}_{LM})$  in which the NonSmoothLaw corresponds to the frictionless unilateral contact. In this case, the problem  $(\mathcal{P}_{LM})$  can be written under the form:

$$\begin{cases} \widehat{M}v_{k+1} + \widehat{f} - HP_{k+1} - G^T \mu_{k+1} = 0 \\ \widehat{G}v_{k+1} = 0 \\ U_{k+1} = H^T v_{k+1} \\ 0 \leq U_{k+1} \perp P_{k+1} \geq 0 \end{cases} \quad (40)$$



## Second order cone

Contrary to the 2D frictional contact problem, the 3D case can not be cast directly into a LCP, because of the non linear nature of the section of the friction cone,  $C(\mu r_n)$

$$C(\mu r_n) = \{ \lambda_t, \sigma(\lambda_t) = \mu r_n - \|\lambda_t\| \geq 0 \} \quad (41)$$

→ Facetization of  $C(\mu r_n)$ .

## Outer approximation

the friction disk  $C(\mu r_n)$  can be approximated by an outer polygon :

$$C_{outer}(\mu r_n) = \bigcap_{i=1}^{\nu} C_i(\mu r_n) \quad \text{with } C_i(\mu r_n) = \{ \lambda_t, \sigma_i(\lambda_t) = \mu r_n - c_i^T \lambda_t \geq 0 \} \quad (42)$$

We now assume that the contact law (??) is of the form

$$-u_t \in N_{C_{outer}(\mu r_n)}(r_t) \quad (43)$$

## Outer approximation

the normal cone to  $C_{outer}(\mu r_n)$  is given by :

$$N_{C_{outer}(\mu r_n)}(r_t) = \sum_{i=1}^{\nu} N_{C_i}(\mu r_n)(r_t) \quad (44)$$

and the inclusion can be stated as:

$$-u_t \in \sum_{i=1}^{\nu} -\kappa_i \partial \sigma_i(\lambda_t), \quad 0 \leq \sigma_i(\lambda_t) \perp \kappa_i \geq 0 \quad (45)$$

Since  $\sigma_i(\lambda_t)$  is linear with the respect to  $\lambda_t$ , we obtain the following LCP :

$$-u_t \in \sum_{i=1}^{\nu} -\kappa_i c_i, \quad 0 \leq \sigma_i(\lambda_t) \perp \kappa_i \geq 0 \quad (46)$$

## Inner approximation

The idea is to approach the friction disk by an interior polygon with  $\nu$  edges. (e.g. Fig.1b)):

$$C_{inner}(\mu r_n) = \{\lambda_t = D\beta, \beta \geq 0, \mu r_n \geq e_T \beta\} \quad (47)$$

where  $e = [1, \dots, 1]^T \in \mathbb{R}^\nu$ , the columns of the matrix  $D$  are the directions vectors  $d_j$  which represent the vertices of the polygon. For the sake of simplicity, we assumed that for every  $i$  there is  $j$  such that  $d_i = -d_j$ .

Following the same process as in the previous case and rearranging the equation, we obtain the following LCP :

$$\begin{cases} r_t = D\beta \\ 0 \leq \beta \perp \lambda e + D^T v_t \geq 0 \\ 0 \leq \lambda \perp \lambda \perp \mu r_n - e_T \beta \geq 0 \end{cases} \quad (48)$$

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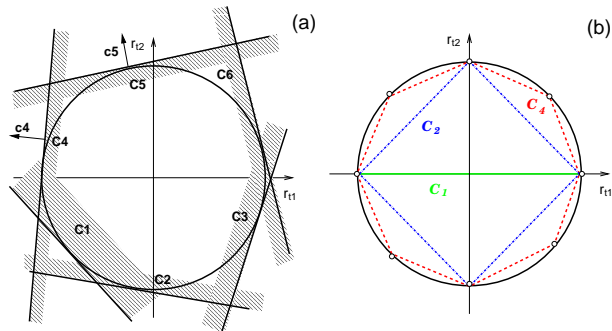


Figure: Approximation of the base of the Coulomb cone by an outer approximation (a) and by an interior  $2\nu$ -gon (b)

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## Comments

- Induced anisotropy in the Coulomb's friction
- The LCP is not necessarily well-posedness

## A direct NCP for the 3D frictional contact.

Let us denote by  $\xi(u_t) = \|u_t\|$  the norm of the tangential velocity, and by  $\sigma(r_t) = \mu r_n - \|r_t\|$  the friction saturation. The problem of contact friction (??) can be easily reformulated into the following NCP:

$$\begin{cases} r_t \xi + \|r_t\| u_t = 0 \\ \xi(u_t) \geq 0, \sigma(r_t) \geq 0, \sigma(r_t) \cdot \xi(u_t) = 0 \end{cases} \quad (49)$$

Two drawbacks are inherent to the previous NCP formulation. Firstly, the NCP formulation is fully nonlinear and it may be difficult to find the well-posed mapping  $F$  of the formulation (19).

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Thank you for your attention.

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