Approaching Optimal Design Problems for Parameterized Variational Inequalities by smooth NLP techniques

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Parameterized Variational Inequalities

Problem: Let $F : \mathsf{R}^{n+m} \to \mathsf{R}^m$, $F \in \mathcal{C}^2$, and $\mathcal{K} \subset \mathsf{R}^m$ be a convex set. Find $y \in \mathsf{R}^m$ such that

$$\langle F(x,y), v - y \rangle \geq 0, \quad \forall v \in \mathcal{K}.$$

x are the design variables, y are the state variables. **Solution set of the variational inequality: $\mathcal{S}(x)$**.

Complementarity Constraint Formulation

Any Parameterized Variational Inequality **(PVI)** can be represented as a problem with complementarity constraints. If $\mathcal{K} = \{ v \in \mathsf{R}^m | \, v \geq b \}$, for some vector $b \in \mathsf{R}^m$, the parameterized variational inequality can be represented as

$$\begin{aligned} F(x, y) &\geq 0, \\ y &\geq b, \\ (y - b)^T F(x, y) &= 0. \end{aligned}$$

Example (Kocvara, Outrata, Zowe, 1998)

Discretization of elastic membrane with rigid obstacle, defined by the mapping $\chi : \Omega(x) \to \mathsf{R}$, $\Omega(x) \subset \mathsf{R}^2$. x **are the design parameters.** Define

$$\begin{aligned} \mathcal{K} &= \left\{ v \in H_0^1\left(\Omega(x)\right) \middle| \, v \geq \chi \text{ a.e. in } \Omega(x) \right\} \\ F(x,u) &= -\Delta u - f \end{aligned}$$

where f is the force perpendicular to the membrane applied to each point (e.g. gravity).

Problem Find the shape of the membrane $u \in \mathcal{K}$ subject to the rigid obstacle constraint:

$$\langle F(x,u), v-u \rangle \geq 0, \quad \forall v \in \mathcal{K}.$$

Most free boundary problems can be expressed like (P)VI!

Optimal Design of PVI

Design parameters x are required to be in set $\mathcal{F}$.

Variational Formulation

$$\begin{array}{rl} \min_{x,u} & \tilde{f}(x,u) \\ \text{subject to} & x \in \mathcal{F} \\ & u \in \mathcal{S}(x) \end{array}$$

Complementarity Formulation

$$\begin{array}{rll} \min_{x,u} & \tilde{f}(x,u) & \\ \text{subject to} & h_i(x) & = 0, i = 1,2,\ldots,n_h \\ & g_j(x) & \leq 0, j = 1,2,\ldots,n_g \\ & F(x,y) & \geq 0, \\ & y - b & \geq 0, \\ (y-b)^T & F(x,y) & = 0. \end{array}$$

For the obstacle problem, we have that $\nabla_y F(x,y)$ is positive definite for any value of x.

Nonsmooth approach

- Applies to the variational approach. If the variational inequality is regular, then $\mathcal{S}(x)$ contains only one point and defines a continuous mapping $y(x)$.
- However, $y(x)$ is **nondifferentiable**, due to the change of the active set with x.
- May use generalized gradients in a bundle trust-region method to solve (Kocvara et al. 1998)

$$\begin{aligned} \min \quad & f(x, y(x)) \\ \text{subject to} \quad & x \in \mathcal{F} \end{aligned}$$

- **Problem: May need a number of computations that grows exponentially in the number of degenerate pairs.**

Nonlinear Programming Approach

Solve the complementarity formulation by a nonlinear programming approach.

Problem: The feasible set has no relative interior, therefore neither will its linearization, because of the complementarity constraints: No constraint qualification.

$$x \leq 0, \ y \leq 0, \ xy = 0 \Rightarrow x, y \text{ cannot both be negative}$$

May be a problem for smooth NLP algorithms (linearization may be infeasible)

Need algorithms that accomodate this type of degeneracy, since all classical algorithms assume that a constraint qualification holds.

Mathematical Programs with Complementarity

Constraints, MPCC

$$
\begin{array}{llll}
\text{minimize}_x & f(x) & & \\
\text{subject to} & g(x) & \leq 0 & \\
 & h(x) & = 0 & \\
 & F_{k1}(x) & \leq 0 & k = 1 \ldots n_c \\
 & F_{k2}(x) & \leq 0 & k = 1 \ldots n_c \\
\text{Compl. constr.} & F_{k1}(x) F_{k2}(x) & = 0 & k = 1 \ldots n_c
\end{array}
$$

Equivalent formulation replaces the equality constraints by (1) $F_{k1}(x)F_{k2}(x) \leq 0$, $k = 1, 2, \ldots K$ or (2) $\sum_{k=1}^{K} F_{k1}(x)F_{k2}(x) \leq 0$. **(M)**

First-order stationarity conditions

$$\begin{aligned}\alpha \nabla_x f(x^*) + \sum_{i=1}^{n_i} \nu_i \nabla_x g_i(x^*) + \sum_{j=1}^{n_e} \pi_j \nabla_x h_j(x^*) \quad + \\ \sum_{k=1}^{n_c} \left[\mu_{k,1} \nabla_x F_{k,1}(x^*) + \mu_{k,2} \nabla_x F_{k,2}(x^*) + \eta_k \nabla_x \left(F_{k,1} F_{k,2} \right)(x^*) \right] \quad = \quad 0\end{aligned}$$

$$\begin{array}{lll} F_{k,i}(x^*) \le 0,\ \mu_{k,i} F_{k,i}(x^*) = 0, & k = 1,2,\ldots,n_c, & i = 1,2 \\ g_i(x^*) \le 0,\ \nu_i \ge 0, & \nu_i g_i(x^*) = 0, & i = 1,2,\ldots,n_i \\ F_{k,1}(x^*) F_{k,2}(x^*) \le 0, & & k = 1,2,\ldots,n_c. \end{array}$$

Plus certain conditions on μ and $\alpha \ge 0$, which determine the nature of the stationarity point !

Types of stationarity points

- **Fritz-John points**: $\alpha \geq 0$, $\mu \geq 0$. Uninteresting, because, by duality, any feasible point is such a point.
- **Clarke-stationary or C-stationary points**: $\alpha = 1$, $\mu_{k,1}\mu_{k,2} \geq 0$ for $k = 1, 2, \ldots, n_c$, whenever $F_{k,1}(x^*) = F_{k,2}(x^*) = 0$.
- **B-stationary** $d = 0$ is a solution of the problem obtained by linearizing evrything **except** the complementarity constraints. Verification of this may require an amount of work that is exponential in the size of the set of degenerate pairs.
- **KKT-stationary or strong stationary points** $\alpha = 1$, $\mu \geq 0$ for $k = 1, 2, \ldots, n_c$.

Nonsmooth Formulation and C-stationarity

$$
\begin{aligned}
\text{minimize}_x \quad & f(x) & & \\
\text{subject to} \quad & g(x) & \leq 0 & \\
& h(x) & = 0 & \\
& \max\{F_{k1} F_{k2}(x)\} & = 0 & \quad k = 1 \ldots n_c
\end{aligned}
$$

The Clarke stationary points are based on this formulation, to which we apply the Clarke stationarity conditions.

Results for MPCC with special structure

$$
\begin{array}{llll}
 & (MPCC) & & \\
\min_{x,y,w,z} & f(x,y,w,z) & & \\
\text{sbj. to} & g(x) & \leq 0 & \\
 & h(x) & = 0 & \\
 & F(x,y,w,z) & = 0 & \\
 & y, w & \leq 0 & \\
 & (y^T w = 0) \;\; y^T w & \leq 0 &
\end{array}
\qquad
\begin{array}{lll}
 & (MPCC(c)) & \\
\min_{x,y,w,z,\zeta} & f(x,y,w,z) + c\zeta & \\
\text{sbj. to} & g(x) & \leq 0 \\
 & h(x) & = 0 \\
 & F(x,y,w,z) & = 0 \\
 & y, w & \leq 0 \\
 & y^T w & \leq \zeta
\end{array}
$$

The elastic mode is used to relax only the complementarity constraints, which are responsible for MFCQ not holding. **We can look at x as design variables and y, w, z as state variables of a parametric variational inequality**.

The P property

We say that a matrix $M \in \mathsf{R}^{n \times n}$ is a P matrix if

$$y = Mx,\ x \neq 0,\ \Rightarrow \exists i,\ 1 \leq i \leq n \text{ such that } x_i y_i > 0$$

We say that the matrix $M \in \mathsf{R}^{(n+m)\times(n+m)}$ has the mixed P property if $x, y \in \mathsf{R}^n$ and $z \in \mathsf{R}^m$

$$\begin{pmatrix} y \\ 0 \end{pmatrix} = M \begin{pmatrix} x \\ z \end{pmatrix},\ x \neq 0 \Rightarrow \exists i,\ 1 \leq i \leq n,\quad \text{such that } x_i y_i > 0$$

Example If B is full column rank and $B^T x = 0$ and $x \neq 0 \Rightarrow x^T A x > 0$, then

$$M = \begin{pmatrix} A & B^T \\ -B & 0 \end{pmatrix}$$

is a mixed P matrix. **Note that A may be indefinite!**

Mixed P partitions

Generalization of mixed *P* matrices. Let $A, B \in \mathsf{R}^{(m+n)\times m}$, $C \in \mathsf{R}^{(m+n)\times n}$. $[A\ B\ C]$ are a mixed P partition if

$$(x, y, z) \neq 0,\ Ax + By + Cz = 0,\ \Rightarrow \exists i,\ x_i y_i > 0$$

Examples M a P matrix $\Rightarrow [I \quad -M]$ is a P partition.

M is a mixed P matrix, $\Rightarrow \begin{bmatrix} I & \\ & -M \\ 0 & \end{bmatrix}$ is a mixed P partition.

Parameterized mixed P variational inequalities

Let $F(x, y, w, z)$ with $F : R^l \times \mathsf{R}^m \times \mathsf{R}^m \times \mathsf{R}^n$ be a continuously differentiable function such that

$$[\nabla_y F \ \nabla_w F \ \nabla_z F]$$

is a mixed P partition **for any** x.

Then the parameterized variational inequality

$$F(x, y, w, z) = 0, \ y^T w = 0$$

has a unique solution for fixed x. In addition, the solution (y, w, z) depends continuously on x.

This framework can accomodate the discretization of the obstacle problem, even when some part of the membrane is glued to the obstacle.

A global convergence result

- Assume that variational inequality satisfies mixed P property (LPR):

$$(\Delta y, \Delta w, \Delta z) \neq 0, \;\; \nabla_y F \Delta y + \nabla_w F \Delta w + \nabla_z F \Delta z = 0 \Rightarrow$$
$$\exists i, \text{ such that } \Delta y_i \Delta w_i > 0.$$

- Assume that the x constraints satisfy MFCQ:

$\nabla h(x)$ is full rank and $\exists u(x)$, $\nabla_x h(x)^T u = 0$, $g_i(x) \geq 0 \Rightarrow \nabla_x g_i(x)^T u < 0$.

- Then **(M)**MPCC(c) satisfies MFCQ everywhere. **An SQP with global convergence (FilterSQP) will accumulate to a feasible stationary point of MPCC(c)**.

- Also, **(M)Any accumulation point** of stationary points $(x(c), y(c), w(c), z(c))$ of MPCC(c) as $c \to \infty$ **is a C-stationary point of MPCC.**! If $\zeta = 0$ for c finite then the point is a **KKT-stationary point** and **the reciprocal holds locally**.

C-stationarity is strictly weaker than KKT!

$$\begin{aligned} \min_{x,y,z} \quad & y - x & & \\ & x & \leq & \ 0 \\ & y + x & = & \ z \\ & y, z & \leq & \ 0 \\ & yz & \leq & \ 0. \end{aligned}$$

This problem has a mixed P submatrix. $(0, 0, 0)$ is the unique minimum but it is not a KKT stationary point. However, it is a C-stationary point.

An elastic mode approach

Choose some $c_0 > 0$, $n = 0$

MPEC1: *Find a solution (stationary point)* $(x^{c_n}, y^{c_n}, w^{c_n}, z^{c_n}, \zeta^{c_n})$ *of (MPEC(*c_n*)).*

If $\zeta^{c_n} = 0$, then $(x^{c_n}, y^{c_n}, w^{c_n}, z^{c_n})$ *solves (MPEC).* Stop.

otherwise *update c:* $c_{n+1} = c_n + K$ *and n:* $n = n + 1$ *and return to* MPEC1

The Tightened Nonlinear Program at a solution x^*

Due to the complementarity constraints, MPCC cannot satisfy MFCQ. But other NLP connected to it can.

TNLP Complementarity constraints are dropped and all active $F_{k,i} \in \mathcal{A}_c(x^*)$ constraints that are part of complementarity pairs are replaced by equality constraints.

$$
\begin{array}{llll}
\text{(TNLP)} \qquad & \min_x & f(x) & \\
& \text{subject to} & g_i(x) \leq 0 & i = 1, 2, \ldots, n_i \\
& & h_j(x) = 0 & j = 1, 2, \ldots, n_e \\
& & F_{\mathcal{A}_c}(x) = 0 &
\end{array}
$$

Sufficient Conditions of KKT stationarity of MPCC

Assume that the tightened nonlinear program TNLP satisfies the strict Mangasarian-Fromovitz constraint qualification SMFCQ at a solution x^* of MPCC, or

1. $\nabla_x F_{\mathcal{A}_c}(x^*)$, and $\nabla_x h(x^*)$ are linearly independent.
2. There exists $p \neq 0$ such that $\nabla_x F_{\mathcal{A}_c}^T(x^*)p = 0$, $\nabla_x h^T(x^*)p = 0$, $\nabla_x g_i^T(x^*)p < 0$, for $i \in \mathcal{A}(x^*)$.
3. The Lagrange multiplier set of TNLP at x^* has a unique element.

Then the Lagrange multiplier set of MPCC is not empty. **MPCC(c) with a finite penalty parameter will also have x^* as a stationary point and it will satisfy MFCQ. Certain elastic mode SQP approaches will stop with a finite parameter.**

Numerical Experiments with SNOPT

Runs done on NEOS for the MacMPEC collection.

Problem	Var-Con-CC	Value	Status	Feval	Elastic
gnash14	21-13-1	-0.17904	Optimal	27	Yes
gnash15	21-13-1	-354.699	Optimal	12	None
gnash16	21-13-1	-241.441	Optimal	7	None
gnash17	21-13-1	-90.7491	Optimal	9	None
gne	16-17-10	0	Optimal	10	Yes
pack-rig1-8	89-76-1	0.721818	Optimal	15	None
pack-rig1-16	401-326-1	0.742102	Optimal	21	None
pack-rig1-32	1697-1354-1	0.751564	Optimal	19	None

MINOS fails on half of these problems.

Results Obtained with MINOS

Runs done with NEOS for the MacMPEC collection.

Problem	Var-Con-CC	Value	Status	Feval	Infeas
gnash14	21-13-1	-0.17904	Optimal	80	0.0
gnash15	21-13-1	-354.699	Infeasible	236	7.1E0
gnash16	21-13-1	-241.441	Infeasible	272	1.0E1
gnash17	21-13-1	-90.7491	Infeasible	439	5.3E0
gne	16-17-10	0	Infeasible	259	2.6E1
pack-rig1-8	89-76-1	0.721818	Optimal	220	0.0E0
pack-rig1-16	401-326-1	0.742102	Optimal	1460	0.0E0
pack-rig1-32	1697-1354-1	N/A	Interrupted	N/A	N/A