



Faculty of Science



Linear Complementarity Problems

A short Introduction to Definitions and Numerical Methods

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The Definition



The Complementarity Problem

If given $x, y \in \mathbb{R}$ where

$$x \geq 0$$

$$y \geq 0$$

and

$$x > 0 \Rightarrow y = 0$$

$$y > 0 \Rightarrow x = 0$$

Then we have a complementarity problem. If for some $a, b \in \mathbb{R}$

$$y = ax + b$$

We have a Linear Complementarity Problem (LCP).



The Linear Complementarity Problem

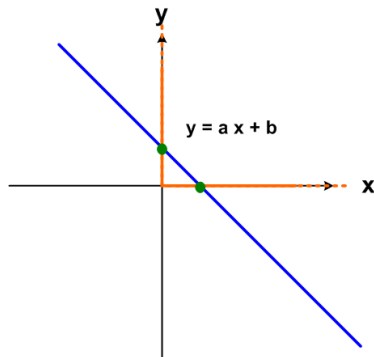
More compact notation

$$x \geq 0$$

$$ax + b \geq 0$$

$$x(ax + b) = 0$$

The Geometry



How many #Solutions of LCP?

Hint: Try to examine signs of a and b

	$b < 0$	$b = 0$	$b > 0$
$a < 0$			
$a = 0$			
$a > 0$			



Answer of # Solutions

Verify this using geometry

	$b < 0$	$b = 0$	$b > 0$
$a < 0$	0	1	2
$a = 0$	0	∞	1
$a > 0$	1	1	1



Going to Higher Dimensions

Let $\mathbf{b}, \mathbf{x} \in \mathbb{R}^n$ and $\mathbf{A} \in \mathbb{R}^{n \times n}$ so $\mathbf{y} = \mathbf{Ax} + \mathbf{b}$,

$$\mathbf{x}_i \geq 0 \quad \forall i \in [1..n]$$

$$(\mathbf{Ax} + \mathbf{b})_i \geq 0 \quad \forall i \in [1..n]$$

$$\mathbf{x}_i(\mathbf{Ax} + \mathbf{b})_i = 0 \quad \forall i \in [1..n]$$

In Matrix-Vector Notation

$$\mathbf{x} \geq 0$$

$$(\mathbf{Ax} + \mathbf{b}) \geq 0$$

$$\mathbf{x}^T(\mathbf{Ax} + \mathbf{b}) = 0$$

How can we solve this?



What kind of problem is a LCP formulation?

What do you think?

- A constrained minimization problem?
- A nonlinear equation (root search problem) ?
- A fixed-point problem?
- A combinatorial problem?
- Something else?



A NAÏVE Active Set/Pivoting Method



Guessing A Solution

Given the index set $\mathcal{I} = \{1, \dots, n\}$ define

$$\mathcal{F} = \{i \mid i \in \mathcal{I} \wedge \mathbf{y}_i > 0\}$$

$$\mathcal{A} = \{i \mid i \notin \mathcal{F} \wedge \mathbf{y}_i = 0\}$$

Make “lucky” guess of \mathcal{F} and \mathcal{A} ,

$$\begin{bmatrix} \mathbf{y}_{\mathcal{A}} \\ \mathbf{y}_{\mathcal{F}} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{\mathcal{A}\mathcal{A}} & \mathbf{A}_{\mathcal{A}\mathcal{F}} \\ \mathbf{A}_{\mathcal{F}\mathcal{A}} & \mathbf{A}_{\mathcal{F}\mathcal{F}} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{\mathcal{A}} \\ \mathbf{x}_{\mathcal{F}} \end{bmatrix} + \begin{bmatrix} \mathbf{b}_{\mathcal{A}} \\ \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$

By assumption $\mathbf{y}_{\mathcal{F}} > 0 \Rightarrow \mathbf{x}_{\mathcal{F}} = 0$

$$\begin{bmatrix} 0 \\ \mathbf{y}_{\mathcal{F}} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{\mathcal{A}\mathcal{A}} & \mathbf{A}_{\mathcal{A}\mathcal{F}} \\ \mathbf{A}_{\mathcal{F}\mathcal{A}} & \mathbf{A}_{\mathcal{F}\mathcal{F}} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{\mathcal{A}} \\ 0 \end{bmatrix} + \begin{bmatrix} \mathbf{b}_{\mathcal{A}} \\ \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$



Verify if Guess was a Solution

So

$$\begin{bmatrix} 0 \\ \mathbf{y}_{\mathcal{F}} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{\mathcal{AA}}\mathbf{x}_{\mathcal{A}} + \mathbf{b}_{\mathcal{A}} \\ \mathbf{A}_{\mathcal{FA}}\mathbf{x}_{\mathcal{A}} + \mathbf{b}_{\mathcal{F}} \end{bmatrix}$$

Compute

$$\mathbf{x}_{\mathcal{A}} = -\mathbf{A}_{\mathcal{AA}}^{-1}\mathbf{b}_{\mathcal{A}}$$

Verify

$$\mathbf{x}_{\mathcal{A}} \geq 0$$

Compute

$$\mathbf{y}_{\mathcal{F}} = \mathbf{A}_{\mathcal{FA}}\mathbf{x}_{\mathcal{A}} + \mathbf{b}_{\mathcal{F}}$$

Verify

$$\mathbf{y}_{\mathcal{F}} > 0$$



How Many Guesses?

We only need

$$\mathbf{A}_{\mathcal{A}\mathcal{A}}^{-1}$$

Hopefully

$$\|\mathcal{A}\| \ll n$$

Cool this will be fast!

How many guesses do we need?



Answer: Non-Polynomial Complexity

Worst case time complexity of guessing

$$\mathcal{O}(n^3 2^n)$$

Not computational very efficient!



Connection to Positive Cones (Linear Programming)

First some algebra on $\mathbf{y} = \mathbf{Ax} + \mathbf{b}$,

$$\mathbf{Iy} = \mathbf{Ax} + \mathbf{b}$$

$$\begin{bmatrix} \mathbf{I} & -\mathbf{A} \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{x} \end{bmatrix} = \mathbf{b}$$

Make guesses $\mathcal{F} = \{i | \mathbf{y}_i \geq 0\}$ and $\mathcal{A} = \{i | \mathbf{x}_i \geq 0\}$ so $\mathcal{F} \cap \mathcal{A} = \emptyset$ and $\mathcal{F} \cup \mathcal{A} = \{1, \dots, n\}$

$$\underbrace{\begin{bmatrix} \mathbf{I}_{\mathcal{F}} & -\mathbf{A}_{\mathcal{A}} \end{bmatrix}}_{\mathbf{M}} \underbrace{\begin{bmatrix} \mathbf{y}_{\mathcal{F}} \\ \mathbf{x}_{\mathcal{A}} \end{bmatrix}}_{\mathbf{z}} = \mathbf{b}$$

Verify if LP

$$\mathbf{Mz} = \mathbf{b} \quad \text{subject to} \quad \mathbf{z} \geq 0$$

Has a solution (same as \mathbf{b} in positive cone of \mathbf{M}).



The Projected Gauss–Seidel Method



Use a Splitting Method

Use the splitting

$$\mathbf{A} = \mathbf{M} - \mathbf{N}$$

then

$$\mathbf{M}\mathbf{x} - \mathbf{N}\mathbf{x} + \mathbf{b} \geq 0$$

$$\mathbf{x} \geq 0$$

$$(\mathbf{x})^T (\mathbf{M}\mathbf{x} - \mathbf{N}\mathbf{x} + \mathbf{b}) = 0$$



Use Discretization \Rightarrow Fixed Point Formulation

Create a sequence of sub problems

$$\mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k \geq 0$$

$$\mathbf{x}^{k+1} \geq 0$$

$$(\mathbf{x}^{k+1})^T (\mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k) = 0$$

where

$$\mathbf{c}^k = \mathbf{b} - \mathbf{N}\mathbf{x}^k$$



Use Minimum Map Reformulation

Given sub problem

$$\mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k \geq 0$$

$$\mathbf{x}^{k+1} \geq 0$$

$$(\mathbf{x}^{k+1})^T (\mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k) = 0$$

Same as (Why?)

$$\underbrace{\min(\mathbf{x}^{k+1}, \mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k)}_{\mathbf{H}(\mathbf{x}^{k+1})} = 0$$

A root search problem: $\mathbf{H}(\mathbf{x}^{k+1}) = 0$.



The Minimum Map Formulation

Say $a, b \in \mathbb{R}$ are complementary

$$a > 0 \Rightarrow b = 0$$

$$b > 0 \Rightarrow a = 0$$

Let us look at the minimum map

$\min(a, b)$	$a > 0$	$a = 0$	$a < 0$
$b > 0$	+	0	-
$b = 0$	0	0	-
$b < 0$	-	-	-

Same solutions as complementarity problem.



More Clever Manipulation

So

$$\min(\mathbf{x}^{k+1}, \mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k) = 0$$

Subtract \mathbf{x}^{k+1}

$$\min(0, \mathbf{M}\mathbf{x}^{k+1} + \mathbf{c}^k - \mathbf{x}^{k+1}) = -\mathbf{x}^{k+1}$$

Multiply by minus one

$$\underbrace{\max(0, -\mathbf{M}\mathbf{x}^{k+1} - \mathbf{c}^k + \mathbf{x}^{k+1})}_{\mathbf{F}(\mathbf{x}^{k+1})} = \mathbf{x}^{k+1}$$

A fixed point formulation: $\mathbf{F}(\mathbf{x}^{k+1}) = \mathbf{x}^{k+1}$.



Do A Case-by-Case Analysis

So

$$\max(0, -\mathbf{M}\mathbf{x}^{k+1} - \mathbf{c}^k + \mathbf{x}^{k+1}) = \mathbf{x}^{k+1}$$

If

$$(-\mathbf{M}\mathbf{x}^{k+1} - \mathbf{c}^k + \mathbf{x}^{k+1})_i \leq 0$$

Then

$$\mathbf{x}_i^{k+1} = 0$$

Else

$$(-\mathbf{M}\mathbf{x}^{k+1} - \mathbf{c}^k + \mathbf{x}^{k+1})_i > 0$$

and

$$(\mathbf{x}^{k+1} - \mathbf{M}\mathbf{x}^{k+1} - \mathbf{c}^k)_i = \mathbf{x}_i^{k+1}$$

That is

$$(\mathbf{M}\mathbf{x}^{k+1})_i = -c_i^k$$



Putting it Together

For suitable choice of \mathbf{M}

$$(\mathbf{M}\mathbf{x}^{k+1})_i = -c_i^k \Rightarrow \mathbf{x}_i^{k+1} = (-\mathbf{M}^{-1}\mathbf{c}^k)_i$$

Back-substitution of $\mathbf{c}^k = \mathbf{b} - \mathbf{N}\mathbf{x}^k$ we have

$$\left(\mathbf{M}^{-1} \left(\mathbf{N}\mathbf{x}^k - \mathbf{b}\right)\right)_i = \mathbf{x}_i^{k+1}$$

Insert in fixed point formulation

$$\underbrace{\max\left(0, \left(\mathbf{M}^{-1} \left(\mathbf{N}\mathbf{x}^k - \mathbf{b}\right)\right)\right)}_{\mathbf{G}(\mathbf{x}^k)} = \mathbf{x}^{k+1}$$

Closed form solution for sub problem: $\mathbf{x}^{k+1} \leftarrow \mathbf{G}(\mathbf{x}^k)$.



Final Iterative Scheme – The Projected Gauss–Seidel (PGS) method

Given \mathbf{x}^1 set $k = 1$

Step 1 Compute

$$\mathbf{z}^k = \left(\mathbf{M}^{-1} \left(\mathbf{N}\mathbf{x}^k - \mathbf{b} \right) \right)$$

Step 2 Compute

$$\mathbf{x}^{k+1} = \max(0, \mathbf{z}^k)$$

Step 3 If convergene then return \mathbf{x}^{k+1} otherwise goto Step 1



Study Group Work

Derive an algebraic equation of the PGS method for the i^{th} component only. That is rewrite

$$\mathbf{x}_i^{k+1} = \max(0, \mathbf{z}_i^k)$$

using $\mathbf{r} = \mathbf{Ax}^k + \mathbf{b}$ and letting

$$\mathbf{M} = \text{diag}(\text{diag}(\mathbf{A})) + \text{tril}(\mathbf{A}, -1)$$

$$\mathbf{N} = -\text{triu}(\mathbf{A}, 1)$$

Here we used Matlab like notation. The final result should only include the terms \mathbf{r}_i , \mathbf{A}_{ii} and \mathbf{x}_i .



The Projected Gauss–Seidel Method...

AGAIN!!!



Connection to Quadratic Programming (QP) Problems

Consider the minimization problem

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \geq 0} \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x}$$

where \mathbf{A} is symmetric. First order optimality (KKT) conditions

$$\mathbf{A} \mathbf{x} + \mathbf{b} - \mathbf{I} \mathbf{y} = 0$$

$$\mathbf{x} \geq 0$$

$$\mathbf{y} \geq 0$$

$$\mathbf{y}^T \mathbf{x} = 0$$

Same as LCP problem.



More on QP relation

From optimization theory we know

- If \mathbf{A} is positive definite then we have a strict convex QP with a unique solution
- If \mathbf{A} is positive semi-definite then we have a convex QP where a solution exist but it is no longer unique

This is cool if we have this prior knowledge¹ of \mathbf{A} .

¹The LCP solution needs not be a global solution of the QP or even a minimizer. It is sufficient that the LCP solution fulfills first-order optimality only.



The QP problem – Again

The LCP problem can be restated as

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \geq \mathbf{0}} f(\mathbf{x})$$

where

$$f(\mathbf{x}) \equiv \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{x}^T \mathbf{b}$$



The Idea – Sweep over Coordinates

The i^{th} unit axis vector

$$\mathbf{e}_j^i = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

The i^{th} relaxation step solves the one dimensional problem

$$\tau^* = \arg \min_{\mathbf{x} + \tau \mathbf{e}^i \geq \mathbf{0}} f(\mathbf{x} + \tau \mathbf{e}^i)$$

and computing $\mathbf{x} \leftarrow \mathbf{x} + \tau \mathbf{e}^i$ same as

$$x_i \leftarrow x_i + \tau$$

One relaxation cycle consist of one sequential sweep over all i 's.



A Closed Form Solution for the i^{th} Coordinate

The object function of the one-dimensional problem

$$\begin{aligned}
 f(\mathbf{x} + \tau \mathbf{e}^i) &= \frac{1}{2}(\mathbf{x} + \tau \mathbf{e}^i)^T \mathbf{A}(\mathbf{x} + \tau \mathbf{e}^i) + (\mathbf{x} + \tau \mathbf{e}^i)^T \mathbf{b}, \\
 &= \underbrace{\frac{1}{2}\tau^2(\mathbf{A})_{ii} + \tau(\underbrace{\mathbf{Ax} + \mathbf{b}}_{\mathbf{r}})_i}_{g(\tau)} + \underbrace{\frac{1}{2}\mathbf{x}^T \mathbf{Ax} + \mathbf{x}^T \mathbf{b}}_{f(\mathbf{x}) \equiv \text{const}}.
 \end{aligned}$$

So

$$f(\mathbf{x} + \tau \mathbf{e}^i) = g(\tau) + f(\mathbf{x})$$

We just need to minimize $g(\tau)$



Found PGS Again

The unconstrained minimizer of $g(\tau)$

$$\tau^u = -\frac{\mathbf{r}_i}{(\mathbf{A})_{ii}}.$$

Considering the constraint $\mathbf{x}_i + \tau \geq 0$ we have

$$\tau^c = \max\left(-\frac{\mathbf{r}_i}{(\mathbf{A})_{ii}}, -\mathbf{x}_i\right)$$

The final update rule

$$\mathbf{x}_i \leftarrow \max\left(0, \mathbf{x}_i - \frac{\mathbf{r}_i}{\mathbf{A}_{ii}}\right)$$

Algebraic equivalent to the i^{th} step in PGS shown by splitting.



Lessons Learned

- PGS can be derived from a QP reformulation or by a splitting method
- Each derivation assumes different matrix properties of the **A**-matrix



Study Group Work

- Show that both derivations end up in algebraic equivalent update formulas for \mathbf{x}_i .
- What properties should the \mathbf{A} have for splitting derivation to work?
- What properties should the \mathbf{A} have for QP derivation to work?
- What properties should the \mathbf{A} have for PGS to converge?
- Speculate what to do if $\mathbf{A}_{ii} \not\geq 0$ (Hint: look at how to minimize $g(\tau)$)?



The Projected Successive Over Relaxation Method



Relaxing the Steps

Given the polynomial

$$g(\tau) \equiv \frac{1}{2}\tau^2 \mathbf{A}_{ii} + \tau \mathbf{r}_i$$

where $\mathbf{A}_{ii} > 0$ then

- One trivial root at $\tau^1 = 0$
- One global minima at $\tau^u = -\frac{\mathbf{r}_i}{\mathbf{A}_{ii}}$ where $g(\tau^0) < 0$
- Second root at $\tau^2 = -2\frac{\mathbf{r}_i}{\mathbf{A}_{ii}}$.

For any τ between τ^1 and τ^2

$$\tau^\lambda = -\lambda \frac{\mathbf{r}_i}{\mathbf{A}_{ii}} \quad \Rightarrow \quad g(\tau^\lambda) < 0, \quad \forall \lambda \in [0..2].$$



The Projected SOR Method

From this it follows that

$$f(\mathbf{x} + \tau^\lambda \mathbf{e}^i) = g(\tau^\lambda) + f(\mathbf{x}) \leq f(\mathbf{x}), \quad \forall \lambda \in [0..2]$$

With equality for $\tau^\lambda = 0$. This results in the over-relaxed version

$$\mathbf{x}_i \leftarrow \max \left(0, \mathbf{x}_i - \lambda \frac{\mathbf{r}_i}{\mathbf{A}_{ii}} \right).$$

Algebraic equivalent to the i^{th} step in the projected SOR².

²PGS is special case when $\lambda = 1$



The Fischer–Newton Method



The Fischer Function

The Fischer function

$$\phi(a, b) = \sqrt{a^2 + b^2} - (a + b) \quad \text{for some } a, b \in \mathbb{R}.$$

If one has the complementarity problem $a \geq 0 \perp b \geq 0$ then a solution (a^*, b^*) is only a solution if and only if $\phi(a^*, b^*) = 0$



The Fischer Reformulation

Given the LCP

$$\mathbf{x} \geq 0 \quad \perp \quad \mathbf{y} = \mathbf{Ax} + \mathbf{b} \geq 0$$

We reformulate

$$\mathbf{F}(\mathbf{x}) = \mathbf{F}(\mathbf{x}, \mathbf{y}) = \begin{bmatrix} \phi(\mathbf{x}_1, \mathbf{y}_1) \\ \vdots \\ \phi(\mathbf{x}_n, \mathbf{y}_n) \end{bmatrix} = \mathbf{0}$$

This is a nonsmooth root search problem



The Fischer–Newton Method

Solved using a generalized Newton–Method. In an iterative fashion solves the generalized Newton subsystem

$$\mathbf{J}\Delta\mathbf{x}^k = -F(\mathbf{x}^k)$$

for the Newton direction $\Delta\mathbf{x}^k$. Here $\mathbf{J} \in \partial F(\mathbf{x}^k)$ is any member from the generalized Jacobian $\partial F(\mathbf{x}^k)$. Then the Newton update yields

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \tau^k \Delta\mathbf{x}^k$$

where τ^k is the step length of the k^{th} iteration.



The Generalized Jacobian

Given \mathbf{F}

- let $\mathcal{D} \subset \mathbb{R}^n$ be the set of all $\mathbf{x} \in \mathbb{R}^n$ where \mathbf{F} is continuously differentiable
- Assume \mathbf{F} is Lipschitz continuous at \mathbf{x}

The B-subdifferential of \mathbf{F} at \mathbf{x} is defined as

$$\partial_B \mathbf{F}(\mathbf{x}) \equiv \{ \mathbf{H} \in \mathbb{R}^{n \times n} \mid \exists (\mathbf{x}_k) \subset \mathcal{D} \text{ and } \lim_{\mathbf{x}_k \rightarrow \mathbf{x}} \frac{\partial \mathbf{F}(\mathbf{x}_k)}{\partial \mathbf{x}} = \mathbf{H} \}$$

Clarke's generalized Jacobian of \mathbf{F} at \mathbf{x} is defined as the convex hull of the B-subdifferential,

$$\partial \mathbf{F}(\mathbf{x}) \equiv \text{co}(\partial_B \mathbf{F}(\mathbf{x}))$$



Example – The Euclidean Norm

Consider the Euclidean norm $e : \mathbb{R}^2 \mapsto \mathbb{R}$ then for $\mathbf{x} \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$ we have

$$\partial e(\mathbf{x}) = \partial_B e(\mathbf{x}) = \frac{\partial e(\mathbf{x})}{\partial \mathbf{x}} = \frac{\mathbf{x}^T}{\|\mathbf{x}\|} \quad \forall \mathbf{x} \neq \mathbf{0}$$

For $\mathbf{x} = \mathbf{0}$ we have

$$\begin{aligned} \partial_B e(\mathbf{0}) &= \{\mathbf{v}^T \mid \mathbf{v} \in \mathbb{R}^2 \text{ and } \|\mathbf{v}\| = 1\} \\ \partial e(\mathbf{0}) &= \{\mathbf{v}^T \mid \mathbf{v} \in \mathbb{R}^2 \text{ and } \|\mathbf{v}\| \leq 1\} \end{aligned}$$



Illustration of Generalized Jacobian in 1D

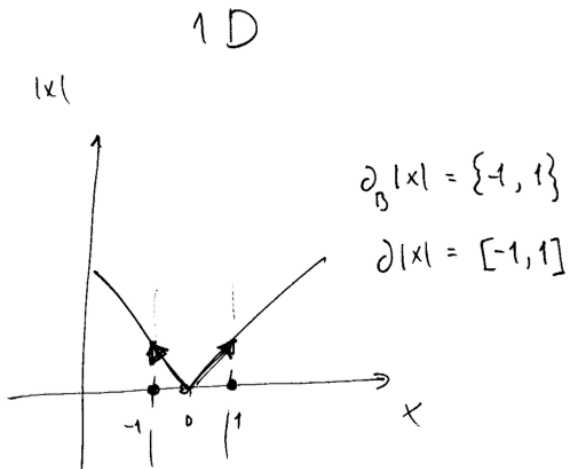
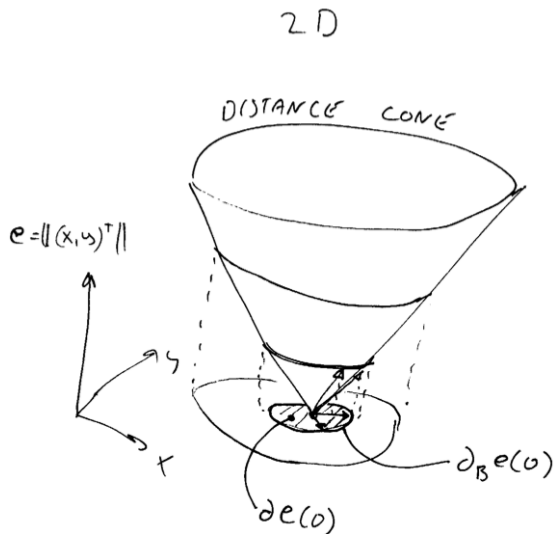


Illustration of Generalized Jacobian in 2D



Example – The Fischer Function

For $\mathbf{x} = [x_1 \ x_2]^T \in \mathbb{R}^2$ we may write the Fischer function as

$$\phi(\mathbf{x}) = e(\mathbf{x}) - f(\mathbf{x})$$

where $f(\mathbf{x}) = \left([1 \ 1]^T \mathbf{x} \right)$. From this we find

$$\partial_B \phi(\mathbf{x}) = \partial_B e(\mathbf{x}) - \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$$

$$\partial \phi(\mathbf{x}) = \partial e(\mathbf{x}) - \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$$

Hence for $\mathbf{x} \neq 0$,

$$\partial \phi(\mathbf{x}) = \partial_B \phi(\mathbf{x}) = \left\{ \frac{\mathbf{x}^T}{\|\mathbf{x}\|} - [1 \ 1]^T \right\}$$

and

$$\partial_B \phi(\mathbf{0}) = \{ \mathbf{v}^T - [1 \ 1]^T \mid \mathbf{v} \in \mathbb{R}^2 \text{ and } \|\mathbf{v}\| = 1 \}$$

$$\partial \phi(\mathbf{0}) = \{ \mathbf{v}^T - [1 \ 1]^T \mid \mathbf{v} \in \mathbb{R}^2 \text{ and } \|\mathbf{v}\| \leq 1 \}$$



Generalized Jacobian of The Fischer Reformulation

Written as

$$\partial F(\mathbf{x}) \equiv \mathbf{D}_p(\mathbf{x}) + \mathbf{D}_q(\mathbf{x})\mathbf{A}$$

where $\mathbf{D}_p(\mathbf{x}) = \text{diag}(p_1(\mathbf{x}), \dots, p_n(\mathbf{x}))$ and

$\mathbf{D}_q(\mathbf{x}) = \text{diag}(q_1(\mathbf{x}), \dots, q_n(\mathbf{x}))$ are diagonal matrices. If $\mathbf{y}_i \neq 0$ or $\mathbf{x}_i \neq 0$ then

$$p_i(\mathbf{x}) = \frac{\mathbf{x}_i}{\sqrt{\mathbf{x}_i^2 + \mathbf{y}_i^2}} - 1,$$

$$q_i(\mathbf{x}) = \frac{\mathbf{y}_i}{\sqrt{\mathbf{x}_i^2 + \mathbf{y}_i^2}} - 1,$$

else if $\mathbf{y}_i = \mathbf{x}_i = 0$ then

$$p_i(\mathbf{x}) = \alpha_i - 1,$$

$$q_i(\mathbf{x}) = \beta_i - 1$$

for any $\alpha_i, \beta_i \in \mathbb{R}$ such that $\| [\alpha_i \quad \beta_i]^T \| \leq 1$



Proof of $\partial F(\mathbf{x})$

Assume $\mathbf{y}_i \neq 0$ or $\mathbf{x}_i \neq 0$ then the differential is

$$d\mathbf{F}_i(\mathbf{x}, \mathbf{y}) = d \left((\mathbf{x}_i^2 + \mathbf{y}_i^2)^{\frac{1}{2}} \right) - d(\mathbf{x}_i + \mathbf{y}_i)$$

By chain rule

$$\begin{aligned} d\mathbf{F}_i(\mathbf{x}, \mathbf{y}) &= \frac{1}{2} (\mathbf{x}_i^2 + \mathbf{y}_i^2)^{-\frac{1}{2}} d(\mathbf{x}_i^2 + \mathbf{y}_i^2) - d\mathbf{x}_i - d\mathbf{y}_i \\ &= \frac{\mathbf{x}_i d\mathbf{x}_i + \mathbf{y}_i d\mathbf{y}_i}{\sqrt{\mathbf{x}_i^2 + \mathbf{y}_i^2}} - d\mathbf{x}_i - d\mathbf{y}_i \\ &= \left[\underbrace{\left(\frac{\mathbf{x}_i}{\sqrt{\mathbf{x}_i^2 + \mathbf{y}_i^2}} - 1 \right)}_{p_i(\mathbf{x})} \quad \underbrace{\left(\frac{\mathbf{y}_i}{\sqrt{\mathbf{x}_i^2 + \mathbf{y}_i^2}} - 1 \right)}_{q_i(\mathbf{x})} \right] \begin{bmatrix} d\mathbf{x}_i \\ d\mathbf{y}_i \end{bmatrix} \end{aligned}$$



Proof of $\partial F(\mathbf{x})$ (Contd)

Finally $d\mathbf{y} = \mathbf{A}d\mathbf{x}$, so $d\mathbf{y}_i = \mathbf{A}_{i*}d\mathbf{x}$ by substitution

$$d\mathbf{F}_i(\mathbf{x}, \mathbf{y}) = \underbrace{\left(p_i(\mathbf{x})\mathbf{e}_i^T + q_i(\mathbf{x})\mathbf{A}_{i*} \right)}_{\partial F_i(\mathbf{x})} d\mathbf{x}$$

The case $\mathbf{x}_i = \mathbf{y}_i = 0$ follows from the previous examples.



How to solve Generalized Newton System

- whenever $\mathbf{x}_i = \mathbf{y}_i = 0$ one would use $\mathbf{x}'_i = \varepsilon$ in-place \mathbf{x}_i when evaluating the generalized Jacobian where $0 < \varepsilon \ll 1$
- If Newton system is solved with iterative method (GMRES) then we only need to compute $\mathbf{J}\Delta\mathbf{x}$. By definition of directional derivative

$$\mathbf{J}\Delta\mathbf{x} = \lim_{h \rightarrow 0^+} \frac{\mathbf{F}(\mathbf{x} + h\Delta\mathbf{x}) - \mathbf{F}(\mathbf{x})}{h}$$

So we can numerically approximate $\mathbf{J}\Delta\mathbf{x}$ using finite differences

- A projected Armijo back-tracking can be very useful to globalize the Newton method and to ensure feasibility of all iterates



Projected Armijo Backtracking Line Search

Define natural merit function

$$\theta(\mathbf{x}) = \frac{1}{2} \mathbf{F}(\mathbf{x})^T \mathbf{F}(\mathbf{x})$$

Project Newton Search Direction

$$\Delta \mathbf{x} \leftarrow \max(\mathbf{0}, \Delta \mathbf{x})$$

Find smallest $k \in \mathbf{Z}_0$ such that

$$\theta(\mathbf{x} + \alpha^k \Delta \mathbf{x}) \leq \theta(\mathbf{x}) + \underbrace{\left(\beta \frac{\partial \theta(\mathbf{x})}{\partial \mathbf{x}} \Delta \mathbf{x} \right)}_{c \equiv \text{const}} \alpha^k$$

for some user defined constants $0 \leq \beta < \alpha < 1$. Now

$$\tau = \alpha^k$$

$$\mathbf{x} \leftarrow \mathbf{x} + \tau \Delta \mathbf{x}$$



Study Group Work

As a challenge if you have time. Derive a Nonsmooth Newton method for the minimum map reformulation of the LCP

$$\min(\mathbf{x}, \mathbf{y}) = \mathbf{0}$$

(Hint: Look at Erleben and Ortiz: A non-smooth newton method for multibody dynamics, In Proc. of ICNAAM 06')



Further Reading

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- D.E. Stewart and J.C. Trinkle. An implicit time-stepping scheme for rigid body dynamics with inelastic collisions and coulomb friction. International Journal of Numerical Methods in Engineering, 39:2673-2691



More Reading

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Study Group Work

- Examine the Stewart–Trinkle (ST) LCP formulation of the contact force problem.
- What matrix properties can you identify?
- What do you know about the right hand side vector?
- What kind of reformulations are applicable to the ST LCP formulation?
- What kind of methods can be used to solve a ST LCP formulation problem?



Basic Programming Exercise

- Obtain Lemke's method from CPNET³
- Create a routine that can generate random N-dimensional LCP problems.
- Generate a sequence of random LCP test problems with increasing number of variables, $N = 2^k$, $k = 2, 3, \dots, 10$.
- Use Lemke to solve random sequences of LCP test problems (run 10 sequences at least).
- Make plots of computing time as a function of increasing number of variables and make a histogram showing the fraction of solved problems.
- Discuss your results – what do you think of Lemke's method?

³<http://www.cs.wisc.edu/cpnet/>



Intermediate Programming Exercise

- Try to implement a PGS solver, a Fischer–Newton solver, and use a QP reformulation solved by using the Matlab **quadprog** function.
- Create a sequence of random problems of increasing size and use the solvers to find solutions.
 - Compare the accuracy of each iterative solver with the true solution, what is the error
 - Plot how the error of each solver behaves as a function of the number of iterations (Hint: make a log plot and determine convergence rate)
 - Try to measure the computing cost per iteration of each solver as a function of increasing variables (Hint: compare plot with your complexity analysis)
- Based on your experiments evaluate if your implementations behave as expected, speculate for what purposes you want to use different solvers for.



Advanced Programming Exercise

Create a simple 2D rigid body simulator using spherical objects of varying size and mass. Ignore friction and use simple first-order time stepping. In each simulation step solve a LCP for the normal penetration constraints.

- Determine the eigenvalue spectrum of the coefficient-matrix
- Determine if the coefficient matrix is symmetric or not
- Try experimenting with using different LCP solvers (take those from the intermediate programming exercise)
- Which solver do you think is best for this particular simulator and why?
- If you have more time try to add friction to the contact forces and rerun all your tests. Did this change on your conclusion on which solver is the best?

