Linear Programming:

Part (i): Strict Feasibility and Degeneracy (Pg 2) Part (ii): Exterior Point Path Following Algorithm (Pg 70)



LP Part (i): Strict Feasibility and Degeneracy

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Tues. Mar. 28, 2023

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Motivation/Main Results

Background

- Currently: simplex and interior point methods are most popular algorithms for solving linear programs, LPs.
- Unlike general conic programs, (finite) LPs do not require strict feasibility for strong duality. Hence strict feasibility is often less emphasized.

We show that lack of strict feasibility:

- causes numerical difficulties in both simplex and interior point methods.
- 2 and \implies all basic feasible solutions, BFS, are degenerate

We present

an extension of Phase-I of simplex method for preprocessing for strict feasibility

Background and Notation

Feasible LPs; standard form (with FINITE opt. value)

$$\begin{array}{ll} (\mathcal{P}) & (\text{finite}) \ p^* = & \min_x & c^T x \\ & \text{s.t.} & Ax = b \in \mathbb{R}^m \\ & x \in \mathbb{R}^n_+ \end{array}$$

assume wlog rank (A) = m;

with feasible set:
$$\mathcal{F} = \{x \in \mathbb{R}^n : Ax = b, x \ge 0\}$$

Dual LP

$$\begin{array}{ll} (\mathcal{D}) \quad p^* = d^* = & \max \quad b^T y \\ & \text{s.t.} \quad A^T y \leq c \in \mathbb{R}^n \\ & y \in \mathbb{R}^m \end{array}$$

(equivalently $A^T y + s = c, s \ge 0$ slack)

History: Kantorovich; Dantzig, Karmarkar

Kantorovich '39, USSR, WWII

- transportation models and optimal solutions (algorithm)
- helped NKVD with transportation problems

Dantzig '47, USA, SIMPLEX METHOD

- following duality/game-theory by Von Neumann
- Hotelling: "but the world is nonlinear"
- Von Neumann: "if you have a linear model, you can now solve it"

• SIAM survey 1970's: 70% of ALL world computer time is spent on the simplex method

Karmarkar '84, Interior Point Revolution

- Lustig-Marsten-Shanno OB1 code '90; large went from: (m = 1e3 × n = 1e4) to (m = 1e5 × n = 1e7)
- to modern day: $(m = 1e6 \times n = 1e10)$

Strict Feasibility, Slater, Mangasarian-Fromovitz CQ

Feasible LPs; standard form (with <u>FINITE</u> opt. value)

$$(\mathcal{P}) \quad \text{(finite)} \ p^* = \min \quad c^T x$$

s.t.
$$Ax = b \in \mathbb{R}^m$$
$$x \in \mathbb{R}^n_+$$

there exists \hat{x} with $A\hat{x} = b, \hat{x} > 0$ (MFCQ)

Dual LP

$$(\mathcal{D}) \quad p^* = d^* = \max_{\substack{b \in \mathcal{D}^T \\ s.t. \\ y \in \mathbb{R}^m}} b^T y \leq c \in \mathbb{R}^n$$

there exists \hat{y} with $A^T \hat{y} < c$ (Slater CQ)

Stability: MFCQ/Slater 4

stability wrt RHS perturbations

↔ compact set of dual variables

Basic (Feasible/Degenerate) Solutions

Definition (basic (feasible) solution)

• Given:
$$x \in \mathbb{R}^n$$
, $Ax = b$ and $\mathcal{B} \subset \{1, ..., n\}$,
 $|\mathcal{B}| = m$; let $\mathcal{N} = \{1 ... n\} \setminus B$.
Then x is a basic solution if

 $A(:, \mathcal{B})$ is nonsingular and $x_i = 0, \forall i \in \mathcal{N}$

x is a basic <u>feasible</u> solution, BFS, if in addition *x* ≥ 0. It is degenerate, if ∃*i* ∈ B, *x_i* = 0

Equivalently, if $Ax = b, x \ge 0$ (feasible):

x is basic if there exists $\mathcal{N} \subset \{1, \dots, n\}, |\mathcal{N}| = n - m, x_i = 0, \forall i \in \mathcal{N};$ and the corresponding matrix of active constraints

$$\begin{bmatrix} A \\ I_{\mathcal{N}} \end{bmatrix}$$
 is nonsingular.

It is degenerate if there are redundant active constraints.

Two Kinds of Degeneracy

Definition (Degenerate BFS)								
x BFS is	{ nondegenerate, degenerate,	if $x_i > 0$, $\forall i \in \mathcal{B}$, otherwise						

Definition (variable fixed at 0)

Let $i_0 \in \mathcal{I} = \{1, \dots, n\}$. x_{i_0} is <u>fixed at 0</u> if $x_{i_0} = 0, \forall x \in \mathcal{F}$. Let

 $\mathcal{I}^{=} = \{i \in \mathcal{I} : x_i \text{ is fixed at } 0\}, \, \mathcal{I}^{<} = \mathcal{I} \setminus \mathcal{I}^{=}$

\bar{x} a degenerate BFS with basis \mathcal{B} is of type:

$$\textbf{if: } i \in \mathcal{B}, \bar{x}_i = \textbf{0} \implies i \in \mathcal{I}^{<}$$

2) if: there exists
$$i \in \mathcal{B} \cap \mathcal{I}^{=}$$

Below we see that: if Type 2 exists, then ALL BFS are of Type 2.

Facial Reduction, FR, for LPs that fail Strict Feasibility

Two Steps

- obtain an equivalent problem with strict feasibility;
- recover full-row rank for the constraint matrix (always needed for MFCQ)

Definition (Face of a convex set K)

A convex set $F \subseteq K \subseteq \mathbb{R}^n$ is a face of K, denoted $F \leq K$, if $y, z \in K, x = \frac{1}{2}(y + z) \in F \implies y, z \in F$. The minimal face for F, face(F), is the intersection of all faces of K containing C.

faces of \mathbb{R}^{n}_{+} , nonnegative orthant

for fixed indices $\hat{\mathcal{I}} \subseteq \{1, \dots, n\}$ $F = \{x \in \mathbb{R}^n_+ : x_i = 0, \forall i \in \hat{\mathcal{I}}\}$

Theorem (DW: [12, Theorem 3.1.3] Theorem of the Alternative)

For the feasible system \mathcal{F} of the LP, exactly one of the following statements holds:

- There exists $x \in \mathbb{R}^{n}_{++}$ with Ax = b, i.e., strict feasibility holds;
- 2 There exists $y \in \mathbb{R}^m$ such that

(*)
$$0 \neq z := A^T y \in \mathbb{R}^m_+$$
, and $\langle b, y \rangle = 0$,

exposing vector $\mathbf{z} \in \mathbb{R}^n_+$

(*) is equivalent to:

exposing vector $0 \neq z \ge 0$ exists for the minimal face containing the feasible set, i.e.,

$$\begin{array}{ccc} x \in \mathcal{F} & \Longleftrightarrow & Ax = b, x \geq 0 \\ & \Longrightarrow & \langle \boldsymbol{z}, x \rangle = \langle \boldsymbol{A}^{\mathsf{T}} \boldsymbol{y}, x \rangle = \langle \boldsymbol{y}, Ax \rangle = \langle \boldsymbol{y}, b \rangle = 0 \end{array}$$

Facial Reduction two steps; Outline

suppose strict feasibility fails; i.e., get exposing vector z

• Thm of Alternative implies: $\exists 0 \leq z = A^T y \in \mathbb{R}^m$:

$$\begin{array}{lll} x \in \mathcal{F} & \Longrightarrow & 0 \leq \langle x, z \rangle = \langle x, A^T y \rangle = \langle Ax, y \rangle = \langle b, y \rangle = 0 \\ & \Longrightarrow & 0 = x \circ z \\ & \Longleftrightarrow & 0 = x_j z_j = 0, \forall j \\ & & \text{yields complementary unit vectors } e_k \end{array}$$

cardinality of support of *z*: $s_z = |\{i : z_i > 0\}|$

Facial Reduction, FR; Two Steps

matrix $V \in \mathbb{R}^{n \times (n-s_z)}$, facial range vector

Every facial reduction step yields at least one redundant constraint, BW: [7],IW: [18, Lemma 2.7],S: [31, Section 3.5].

Lemma (step 2: redundant constraint)

Consider the facially reduced feasible set

$$\mathcal{F}_r = \left\{ \mathbf{v} : \mathbf{AVv} = \mathbf{b}, \mathbf{v} \in \mathbb{R}^{n-s_z}_+ \right\}.$$

Then at least one linear constraint of the LP is redundant.

Proof.

Let: $0 \neq z = A^T y \ge 0$ exposing vector; V corresponding facial range vector; Then:

 $0 = V^T z = V^T A^T y = (AV)^T y = \sum_{i=1}^m y_i ((AV)^T)_i$ Since $0 \neq y \in \mathbb{R}^m$, the rows of AV are linearly dependent.

Summary FR

Result of full two step FR: strict feas.; full rank

$$\mathcal{F} = \{ x \in \mathbb{R}^n_+ : Ax = b \}$$

=
$$\{ x = Vv \in \mathbb{R}^n : \overline{A}v := (P_{\overline{m}}AV)v = (P_{\overline{m}}b) =: \overline{b},$$

$$v \in \mathbb{R}^{n-s_2}_+ \}$$

- after substit: $\min(V^T c)^T v$ s.t. $\bar{A}v = \bar{v}, v \in \mathbb{R}^{n-s_z}_+$
- $\exists \hat{\mathbf{v}} > \mathbf{0}, \bar{A}\hat{\mathbf{v}} = \bar{b}$ (MFCQ)
- full rank $\overline{A} = P_{\overline{m}}AV$: $P_{\overline{m}} : \mathbb{R}^m \to \mathbb{R}^{\overline{m}}$, $\overline{m} = \operatorname{rank}(AV) < m$. $P_{\overline{m}}$ is projection that chooses the linearly independent rows of AV.
- BOTH # variables, # constraints are strictly reduced.

This emphasizes the ILL-CONDITIONING of problems where strict feasibility fails, i.e., Implicit singularity is eliminated using FR.

Facial Reduction, FR

a journey to reformulate a problem until strict feasibility is met

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,

Solve the auxiliary system:

Find
$$y \in \mathbb{R}^m$$
 s.t. $A^T y \in \mathbb{R}^n_+ \setminus \{0\}$
 $\langle b, y \rangle = 0$
Set $V = I(:, \operatorname{supp}(A^T y)^c)$
 $x \leftarrow Vv$
 $\mathcal{F} \leftarrow \{v \ge 0 : (AV)v = b\}$

Facial Reduction, FR

a journey to reformulate a problem until strict feasibility is met

[STEP 1] Solve the auxiliary system:

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[STEP 2] Any nontrivial FR ↓ discovery of redundant equalities

Use $P_{\bar{m}}$ to discard redundancies

$$\mathcal{F} \leftarrow \{ v \geq 0 : P_{\bar{m}}AV(v) = P_{\bar{m}}b \}$$

Facial Reduction, FR

a journey to reformulate a problem until strict feasibility is met

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Example

Consider \mathcal{F} with the data

$$A = \begin{bmatrix} 1 & 1 & 3 & 5 & 2 \\ 0 & 1 & 2 & -2 & 2 \end{bmatrix} \text{ and } b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Set $y = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \implies A^T y = \begin{pmatrix} 1 & 0 & 1 & 7 & 0 \end{pmatrix}^T \ge 0 \text{ and } \langle b, y \rangle = 0.$
$$V = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad x \leftarrow Vv = \begin{pmatrix} 0 \\ v_1 \\ 0 \\ v_2 \end{pmatrix}, \quad Ax = b \leftarrow AVv = b \equiv \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix} v = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

(*) Side note

There are exactly six feasible bases in \mathcal{F} ; (BFS all degenerate).

•
$$\mathcal{B} \in \{\{1,2\},\{2,3\},\{2,4\}\}$$
 is $x = \begin{pmatrix} 0 & 1 & 0 & 0 \end{pmatrix}^{T};$

• $\mathcal{B} \in \{\{1,5\}, \{3,5\}, \{4,5\}\}$ is $x = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}^T$.

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Lemma (AV is rank deficient)

Consider the facially reduced feasible set

$$\mathcal{F}_r = \left\{ \mathbf{v} : \mathbf{AVv} = \mathbf{b}, \mathbf{v} \in \mathbb{R}^{n-s_z}_+ \right\}.$$

Then at least one linear equality of AVv = b is redundant.

(proof) Let $z = A^T y$ be the exposing vector, V be a facial range vector induced by z. Then

$$0 = V^T z = V^T A^T y = (AV)^T y.$$

Found a nontrival row combination of AV, i.e., detected redundancy

Definition (implicit problem singularity)

The implicit problem singularity (ips) = The number of implicit redundant equalities of ${\cal F}$

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Singularity Degree $sd(\mathcal{F})$, Sturm '20 [32]

Definition ($d = sd(\mathcal{F}) = \min |FR \ steps|$)

Definition (Hölder regularity)

the pair of closed, convex subsets A, B is γ -Hölder regular if $\forall U$ compact, $\exists c > 0$ with: dist $(x, A \cap B) \leq c \cdot (dist^{\gamma}(x, A) + dist^{\gamma}(x, B))$ for all $x \in U$.

Sturm [32] error bound Theorem for SDP, $\mathcal{F} = \mathcal{L} \cap \mathbb{S}^n_+$

 $(\mathcal{L}, \mathbb{S}^n_+)$ is $\frac{1}{2^d}$ -Hölder regular. (\mathcal{L} linear manifold)

for LPs, FR in *one* iteration using maximal exposing vector,
i.e., *d* = sd(*F*) ≤ 1
FR for LPs does not alter sparsity pattern of *A*. (only involves discarding columns of *A*; rows of *A*, *b*)

Theorem

^a Suppose that strict feasibility of \mathcal{F} fails. Then every basic feasible solution, BFS, $x \in \mathcal{F}$ with basis \mathcal{B} has $\mathcal{B} \cap \mathcal{I}^{=} \neq \emptyset$ and thus is degenerate.

^aContrapositive found in Bertsimas-Tsitsiklis book [4, Exer. 2.19].

Proof.

- $\mathcal{F} = \{x \in \mathbb{R}^n : AVv = b, v \in \mathbb{R}^{n-s_z}_+\}, \text{ facial range vctr } V$ • wlog $V = \begin{bmatrix} I_r \\ 0 \end{bmatrix}$ and $r = n - s_z$;
- recall by redundant constraint lemma: rank AV < m
- implies rank $A(:, \{1, ..., r\}) < m$
- BFS implies rank $A(:, \mathcal{B}) = m$; implies $\exists i \in \mathcal{B}, i > r$
- implies $\exists i \in \mathcal{B} \cap \mathcal{I}^{=}, x_i = 0$ (degeneracy)

Corollary (contrapositive motivates phase I part 2)

If there exists a nondegenerate basic feasible solution, then there exists a strictly feasible point in \mathcal{F} .

Stability from above corollary

Recall: strict feasibility (and full rank, MFCQ) is equivalent to stability wrt RHS perturbations.

Example (converse fails; all BFS degenerate \implies MFCQ fails)

 $A = \begin{bmatrix} 1 & 0 & 2 & 0 & -2 \\ 1 & -3 & 2 & 1 & -2 \end{bmatrix}; b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad 0 < x = \frac{1}{10} \begin{pmatrix} 1 & 1 & 5.5 & 3 & 1 \end{pmatrix}^{T}$ 4 deg. feas. bases: $\mathcal{B} = \{\{1,2\},\{1,4\}: x = (1,0,0,0,0)^{T}$ $\mathcal{B} = \{2,3\},\{3,4\}: x = (0,0,1/2,0,0)^{T}$

(Also, the linear assignment problem is highly degenerate but has a strictly feasible point (average).)

We want to avoid implicit singularity

• improve conditioning, number of iterations

interior point methods

- Condition number of normal equation system
- stopping criteria

$$\mathsf{KKT} = \left(\frac{\|\mathbf{A}\mathbf{x}^* - \mathbf{b}\|}{1 + \|\mathbf{b}\|}, \ \frac{\|\mathbf{A}^T\mathbf{y}^* + \mathbf{s}^* - \mathbf{c}\|}{1 + \|\mathbf{c}\|}, \ \frac{\langle \mathbf{x}^*, \mathbf{s}^* \rangle}{n}\right).$$

simplex methods (NETLIB data set)

• percentage of degenerate iterations

Interior Point Methods

Optimality Conditions at current (x > 0, y, s > 0), $\mu > 0$

X = Diag(x), S = Diag(s).

$A' \Delta y + \Delta s - c$	=	0	dual feasibility
$A\Delta x - b$	=	0	primal feasibility
$S \Delta x + X \Delta s$	=	$\mu oldsymbol{e}$	complementary slackness

After block elimination, solve normal equations for Δy

- Use Δs in eqn 1 to eliminate Δs in eqn 3.
- Solve for Δx in eqn 3 and eliminate it in eqn 2.
- We get the normal equations

$$AS^{-1}XA^{T}\Delta y = RHS.$$

• Backsolve for Δx , Δs to get the Newton direction.

Numerical Experiments with Interior Point Methods

condition numbers of normal matrix; x^* , s^* near optimal

$$\kappa\left(AD^*A^T\right)$$
, where $D^* = \text{Diag}\left(x^*\right)\text{Diag}\left(s^*\right)^{-1}$ (1)

three families of instances

- ($\mathcal{P}_{(A,b,c)}$) do not have strictly feasible points;
- ($\bar{\mathcal{P}}_{(A,\bar{b},c)}$) have strictly feasible points;
- ($\mathcal{P}_{(A_{FR}, b_{FR}, c_{FR})}$) facially reduced instances of $(\mathcal{P}_{(A, b, c)})$.

Condition Numbers of Normal Matrix Near Optimum



Figure: Performance profile on κ (*ADA*^T) with(out) strict feasibility near optimum; various solvers

test the average performance of 10 instances of size (n, m, r) = (3000, 500, 2000)

$KKT = \left(\frac{\ Ax^* - b\ }{1 + \ b\ }, \ \frac{\ A^T y^* + s^* - c\ }{1 + \ c\ }, \ \frac{\langle x^*, s^* \rangle}{n}\right)$									
			Non-Facially Reduced System	Facially Reduced System					
		KKT	(9.58e-16, 1.80e-12, 5.17e-09)	(5.78e-16, 1.51e-15, 5.57e-08)					
	linprog iter		23.30	17.60					
		time	1.10	0.76					
	KKT		(1.51e-10, 1.49e-12, 4.67e-03)	(8.54e-12, 3.75e-16, 4.19e-06)					
	SDPT3	iter	25.40	19.80					
		time	0.82	0.53					
KKT		KKT	(8.40e-09, 7.54e-16, -5.16e-06)	(5.16e-09, 3.81e-16, -2.03e-08)					
	MOSEK	iter	35.90	10.10					
		time	0.58	0.31					

Table: Average of KKT conditions, iterations and time of (non)-facially reduced problems

Numerical Experiments with (Dual) Simplex Method

Empirics on the Number of Degenerate Iterations

• MOSEK (values in the table) reports percentage of degenerate iterations i.e., 'DEGITER(%)' is ratio of degenerate iterations. (smaller value is better).

• $r = |\operatorname{supp}(s)|$; smaller value (r/n)% means entries of *s* are identically 0; 100% means strict feasibility holds.

• note significant decrease in 'DEGITER(%)'.

			((<i>r</i> / <i>n</i>)%		
		60%	70%	80%	90%	100%
	(1000, 250)	36.62	10.18	0.01	0.02	0.00
(n,m)	(2000, 500)	39.72	18.28	0.07	0.15	0.01
(11, 111)	(3000, 750)	25.99	10.66	0.32	0.75	0.02
	(4000, 1000)	29.78	18.25	0.25	0.53	0.02

Table: Average of ratio of degenerate iterations DEGITER(%)

Phase I(b): Towards Strict Feasibility

$$p_1^* = \max\{x_1 : Ax = b, x \ge 0\}.$$

- Suppose that p^{*}₁ > 0. Then, the the variable x₁ is not an identically 0 variable, i.e., 1 ∉ I₀.
- Suppose that p^{*}₁ = 0. Then, the variable x₁ is an identically 0 variable, i.e., 1 ∈ I₀. Let B^{*} be an optimal basis. Then we have an exposing vector

$$y^* = A(:, \mathcal{B}^*)^T e_1, \ \langle b, y^* \rangle = 0 \ \text{ and } A^T y^* \ge e_1.$$

• Add up certificates: $y^{\circ} = \sum_{j} y^{j}$ to get exposing vector

$$\mathcal{A}^T \mathbf{y}^\circ = \sum_j \mathcal{A}^T \mathbf{y}^j \ge \mathbf{0}, \mathcal{A}^T \mathbf{y}^\circ \ne \mathbf{0}, \langle \mathbf{b}, \mathbf{y}^\circ
angle = \sum_j \langle \mathbf{b}, \mathbf{y}^j
angle = \mathbf{0}.$$

- loss of strict feasibility has many applications recent survey Drusvyatskiy-W. [12].
- though not needed theoretically in LP, loss of MFCQ results in stability/numerical issues.
- In the paper we introduced new concept: Implicit Singularity Degree, maximum number of FR steps, and presented an algorithm, phase I (b), that regularizes an LP, for strict feasibility holding.

Regularized Nonsmooth Newton Algorithms for Best Approximation with Applications



Tues. Mar. 28, 10:00-11:20 EST, 2023

joint work with: Yair Censor (Univ. of Haifa); Walaa Moursi and Tyler Weames (Univ. of Waterloo)

Main Problem/Best Approximation

Given $v \in \mathbb{R}^n$ and $P \subset \mathbb{R}^n$ a polyhedral set, find the nearest point to *v* from the set *P*

Nonsmooth Algorithms

- Application of Moreau Decomposition/elegant equation
- present regularized nonsmooth method; singular Jacobian
- compare computational performance to classical projection methods (e.g., HLWB projection method)

Applications

solving large scale linear programs; triangles from branch and bound methods; generalized constrained linear least squares.

Notation

best approximation problem to polyhedral set $P \subset \mathbb{R}^n$

find the nearest point $x^* \in P$ to a given point $v \in \mathbb{R}^n$

uniquely attained optimum (projection of v onto P)

optimum:
$$x^*(v) = \operatorname{argmin}_{x \in P} \frac{1}{2} ||x - v||^2$$

optimal value:
$$p^*(v) = \frac{1}{2} ||x^*(v) - v||^2$$

Nonsmooth Newton Method

We apply a (regularized/scaled) nonsmooth Newton method to a special form of the optimality conditions based on a Moreau decomposition.

Background

- The special Moreau decomposition for the optimality conditions comes from work in infinite dimensional Hilbert space e.g., [9, 10, 23, 8], where the projection is actually differentiable, and typically *P* is the intersection of a cone and a linear manifold of finite co-dimension (finite # constraints).
- parametrized quadratic problem to solve finite dimensional linear programs [30] applied in our work here below. (In this finite dimensional case differentiability was lost.)
- infinite dimensional applications appear in the theory of *partially finite programs* in [5,6] Further references in [29, 19, 2].

Semismoothness

- differentiability is lost in finite dimensional; this led to application of semismoothness [24, 26, 25].
- More recently: applications for nearest Euclidean distance matrices and nearest doubly stochastic in [1, 17].
- The optimum *x**(*v*) is often called the *projection onto the polyhedral set* and is known to be unique. Differentiability properties are nontrivial as discussed in e.g., [16]. A characterization of differentiability in terms of normal cones is given in [13]. Further results and connections to semismoothness is in e.g., [16, 15]. A survey presentation is at [28].

Projection onto a Polyhedral Set

Assumptions: A full row rank; feasible set nonempty

Optimality Conditions

Theorem ($F : \mathbb{R}^m \to \mathbb{R}^m$; find root y^* ; Newton)

The optimum $x^*(v)$ exists and is unique. Let (*) $F(y) := A(v + A^T y)_+ - b$, $f(y) := \frac{1}{2} ||F(y)||^2$ Then F(y) = 0 has a root y^* , $F(y^*) = 0 \iff y \in \operatorname{argmin} f(y^*)$

 $x^*(v) = (v + A^T y^*)_+$, for any root $F(y^*) = 0$.

Moreover, strong duality holds and the dual problem is

$$p^{*}(v) = d^{*}(v)$$

:= $\max_{z \ge 0, y} \phi(y, z) \quad (= \min_{x} L(x, y, z))$
:= $-\frac{1}{2} ||z - A^{T}y||^{2} + y^{T}(Av - b) - z^{T}v.$

AND

At each iteration, we get a provable/calculable lower bound

$$\max_{z \ge 0, y} \phi(y, z) = -\frac{1}{2} \left\| z - A^T y \right\|^2 + y^T (Av - b) - z^T v$$

Proof of Optimality Conditions

Proof.

$$L(x, y, z) = \frac{1}{2} ||x - v||^2 + y^T (b - Ax) - z^T x;$$

$$\nabla_x L(x, y, z) = x - v - A^T y - z;$$

stationarity: $0 = \nabla_x L(x, y, z) \implies x = (v + A^T y) + z$

$$\implies L(x, y, z) = -\frac{1}{2} ||z + A^T y||^2 + y^T (b - Av) - z^T v.$$

KKT optimality conditions

$$\begin{array}{rcl} \frac{\partial}{\partial x}L(x,y,z) &=& x-v-A^{T}y-z &=& 0 \quad (\text{dual feasibility})\\ \frac{\partial}{\partial y}L(x,y,z) &=& Ax-b &=& 0 \quad (\text{primal feasibility})\\ \frac{\partial}{\partial z}L(x,y,z) &\cong& x \in (\mathbb{R}^{n}_{+}-z)^{+} & (\text{compl. slackness,}\\ && z^{T}x = 0 \text{ or}\\ && z \circ x = 0) \end{array}$$

Proof continued...

(cont... Solve opt. cond.

$$\begin{bmatrix} x - v - A^T y - z \\ Ax - b \\ z^T x \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad X, Z \in \mathbb{R}^n_+, Y \in \mathbb{R}^m.$$

Moreau Decomposition: $v + A^T y = x - z = x + (-z), x^T z = 0$ $x = (v + A^T y)_+; z = -(v + A^T y)_-$

$$F: \mathbb{R}^m \to \mathbb{R}^m; \quad F(y) = A(v + A^T y)_+ - b = 0, \ y \in \mathbb{R}^m$$

Apply Newton at current y_c ; Newton direction Δy

 $F'(y_c)\Delta y = -F(y_c);$ $y_p = y_c + \Delta y$

Compare Interior Point Methods

Block Elimination on Perturbed KKT Conditions

$$\begin{bmatrix} {}^{r_d}_{r_p} \\ {}^{r_p}_{r_c} \end{bmatrix} := \begin{bmatrix} x - v - A^T y - z \\ Ax - b \\ Zx - \mu \theta \end{bmatrix}, \quad \mathbf{X}, \mathbf{Z} \in \mathbb{R}^n_+, \mathbf{y} \in \mathbb{R}^m.$$
$$F'_{\mu} \Delta \mathbf{s} = \begin{bmatrix} \Delta \mathbf{x} - A^T \Delta y - \Delta z \\ A\Delta x - b \\ X\Delta z + Z\Delta x \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} = - \begin{bmatrix} {}^{r_d}_{r_p} \\ {}^{r_p}_{r_c} \end{bmatrix}, \quad \mathbf{X}, \mathbf{Z} \in \mathbb{R}^n_+, \mathbf{y} \in \mathbb{R}^m.$$

Normal Equations Reduction to Δy

Currently, normal equations are not considered efficient. But the Newton equation was a percursor and appears to be efficient?

$$F: \mathbb{R}^m \to \mathbb{R}^m; \quad \Big| F(y) = A(v + A^T y)_+ - b = 0, \ y \in \mathbb{R}^m \Big|$$

 $F'(y_c)\Delta y = -F(y_c);$ $y_p = y_c + \Delta y$

minimize squared residual $f(y) = \frac{1}{2} ||F(y)||^2$

differentiable case
$$\{i : (v + A^T y)_i = 0\} = \emptyset$$
:
 $\nabla f(y) = (F'(y))^* F(y)$

Definition ((local) Lipschitz Continuity)

Let $\Omega \subseteq \mathbb{R}^n$. A function $F : \Omega \to \mathbb{R}^n$ is *Lipschitz continuous* on Ω if there exists K > 0 such that

$$|F(y) - F(z)| \le K ||y - z||, \forall y, z \in \Omega.$$

F is *locally Lipschitz continuous* on Ω if for each $x \in \Omega$ there exists a neighbourhood *U* of *x* such that *F* is Lipschitz continuous on *U*.

Rademacher's Theorem [27, 14]

 $F: \Omega \to \mathbb{R}^n$ locally Lipschitz on Ω implies that it is Frechét differentiable almost everywhere on Ω .

Definition (Clarke [11] Generalized Jacobian)

Suppose that $F : \mathbb{R}^m \to \mathbb{R}^m$ be locally Lipschitz. Let D_F be the set of points such that F is differentiable. Let F'(y) be the usual Jacobian matrix at $y \in D_F$. The *generalized Jacobian of F at y*, $\partial F(y)$ is

$$\partial F(y) = \operatorname{conv} \left\{ \lim_{\substack{y_i o y \\ y_i \in D_F}} F'(y_i)
ight\}.$$

In addition, $\partial F(y)$ is nonsingular if every $V \in \partial F(y)$ is nonsingular.

Case: Differentiable and F'(y) invertible

Newton Direction; Newton Equation

$$(F'(y))^*(F'(y))\Delta y = -(F'(y))^*F(y) \iff F'(y)\Delta y = -F(y).$$

$$\Delta y = -\left((F'(y))^*(F'(y))\right)^{-1}(F'(y))^*F(y) = -(F'(y))^{\dagger}F(y)$$

directional derivative: $\Delta y^T \nabla f(y) = \dots$

$$- [(F'(y))^*F(y)]^T ((F'(y))^*(F'(y)))^{-1} [(F'(y))^*F(y)] < 0$$

Levenberg-Marquardt, LM, Regularization Method

We now see that we maintain a descent direction.

Lemma (for handling singularity in $(F'(y))^*(F'(y))$)

LM direction is always a descent direction.

Proof.

 $(J \cong F'(y))$

$$(J^*J + \lambda I)\Delta y = -J^*F.$$

 $\Delta y = -(J^TJ + \lambda I)^{-1}(J^TF)$

Therefore, the directional derivative is

$$\Delta y^{T} \nabla f(y) = -\left(\left(J^{T} J + \lambda I \right)^{-1} \left(J^{T} F \right) \right)^{T} \left(J^{T} F \right)$$

= $- \left(J^{T} F \right)^{T} \left(\left(J^{T} J + \lambda I \right)^{-1} \right) \left(J^{T} F \right)$
< 0.

Max. Rank Generalized Jacobian

Cols chosen \cong pos. variables of *w*

$$Aw_+ = A(\mathcal{P}_{\mathcal{N}}w) = (A\mathcal{P}_{\mathcal{N}})w_+ = \sum_{w_i>0} A(:,i)w_i$$

Index Set of Columns

Note:
$$v + A^T y \ge 0 \implies F'(\Delta y) = A A^T \Delta y = A A^T \Delta y$$

$$\mathcal{U}(y) := \left\{ \begin{array}{ll} u \in \mathbb{R}^n \mid u_i \in \left\{ \begin{array}{cc} 1 & \text{if } (v + A^T y)_i > 0\\ [0,1] & \text{if } (v + A^T y)_i = 0\\ 0 & \text{if } (v + A^T y)_i < 0 \end{array} \right\} \right\}$$

generalized Jacobian at y; after convex hull

 $\partial F(y) = \{A \operatorname{Diag}(u) A^T | u \in \mathcal{U}(y)\}$ (max-rank: choose $u_i = 1$ when possible)

Semismooth Newton Method solving F(y) = 0

Solve
$$(V_k + \lambda I)d_{Newton} = -F(y^k)$$
, with
 $V_k \in \partial F(y^k), \lambda > 0, c \in (0, 1)$
 $y^{k+1} = y^k + d_{Newton}$; (or avging $y^{k+1} = (1 - c)y^k + +cd_{Newton}$)

Max-rank Jacobian

$$\begin{array}{lll} AMA^{T} & := & A\text{Diag}\left(u\right)A^{T} \\ & = & \sum_{i \in \mathcal{I}_{+}} A_{:i}A_{:i}^{T} + \sum_{i \in \mathcal{I}_{0}} \alpha_{i}A_{:i}A_{:i}^{T}, \, \alpha_{i} \in [0,1], \forall i \in \mathcal{I}_{0} \end{array}$$

maximum (resp. minimum) rank for AMA: $\alpha_i = 1, \forall i \in \mathcal{I}_0 \ (\alpha_i = 0, \forall i \in \mathcal{I}_0, \text{ resp.})$

Choosing the optima for the tests; (nondegenerate) vertex

In our tests we can decide on the characteristics of the optimal solution using the properties of (degenerate) vertices. Recall: *x* optimal iff $x - v \in \mathcal{F}(x)^+$

Lemma (vertex and polar cone)

 $y \in \mathbb{R}^{m}, x(y) = (v + A^{T}y)_{+} \in \mathcal{F}.$ Then: x(y) vertex $\iff A_{\mathcal{I}_{+}}$ nonsingular \iff corresp. gen. Jac. nonsingular. $x = x(y) \in \mathcal{F} \implies$ $\mathcal{F}(x)^{+} = \{w : w = A^{T}u + z, u \in \mathbb{R}^{m}, z \in \mathbb{R}^{n}_{+}, x^{T}z = 0\}$

Proof of Lemma

Proof.

wlog
$$A = [A_{\mathcal{I}_+} A_{\mathcal{I}_0}]$$
 implies active set is

$$\begin{bmatrix} A_{\mathcal{I}_+} & A_{\mathcal{I}_0} \\ 0 & I \end{bmatrix} x = \begin{pmatrix} b \\ 0 \end{pmatrix};$$

This has unique solution x(y) iff $A_{\mathcal{I}_+}$ is nonsingular. gradient of objective satisfies

$$x-v=A^Ty+\sum_{j\in\mathcal{I}_0}z_je_j.$$

Optimality conditions yield polar cone at a vertex.

degeneracy of optimal solutions

Let $x \in bdry \mathcal{F}$; x is optimal iff $x - v \in \mathcal{F}(x)^+$, i.e., we can choose v with $v = x - A^T u + z$, $z \ge 0$, $z^T x = 0$. and $x^*(v)$ is differentiable at $v \iff (x^*(v) - v) \in ri(\mathcal{F} - x^*(v))^+$

Best Approx.; Nonsmooth Algor.

Algorithm 1 Best Approx. of v in P; Exact Newton

Require: $v \in \mathbb{R}^n$, $y_0 \in \mathbb{R}^m$, $(A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = m)$, $\varepsilon > 0$, maxiter 1: **Output.** Primal-dual opt: x_{k+1} , (y_{k+1}, z_{k+1}) 2: Initialization. $k \leftarrow 0, x_0 \leftarrow (v + A^T y_0)_+, z_0 \leftarrow (x_0 - (v + A^T y_0))_+,$ $F_0 = Ax_0 - b$, stopcrit $\leftarrow ||F_0||/(1 + ||b||)$ 3: while ((stopcrit > ε) & ($k \le$ maxiter)) do 4: $\lambda = \min(1e^{-3}, \text{ stopcrit})$ 5: $\bar{V} = (V_k + \lambda I_m)$ solve pos. def. $Vd = -F_k$ for Newton direction d 6: updates 7: 8: $y_{k+1} \leftarrow y_k + d$ $x_{k+1} \leftarrow (v + A^T y_{k+1})_+$ 9: 10: $Z_{k+1} \leftarrow (X_{k+1} - (V + A^T V_k))_{\perp}$ 11: $F_{k+1} \leftarrow Ax_{k+1} - b$ (residual) 12: stopcrit $\leftarrow \|F_{k+1}\|/(1+\|b\|)$ $k \leftarrow k + 1$ 13: 14: end while

Halpern-Lions-Wittmann-Bauschke [3]

Halpern-Lions-Wittmann-Bauschke [3]

(HLWB)

Algorithm 2 Extended HLWB algorithm

Require: $v \in \mathbb{R}^n$, $(A \in \mathbb{R}^{m \times n}, \operatorname{rank}(A) = m)$, $\varepsilon > 0$, maxiter $\in \mathcal{N}$. 1: Output. x_{k+1} **2:** Initialization. $k \leftarrow 0$, msweeps $\leftarrow 0 x_0 \leftarrow max(v, 0), y_0 \leftarrow x_0, i_0 = 1$ stopcrit $\leftarrow ||Ay_0 - b||/(1 + ||b||) (= ||F_0||/(1 + ||b||))$ **3:** while ((stopcrit > ε) & ($k \le$ maxiter)) do 4: if 1 < i(k) < m then $y_k = x_k + \frac{b_{i_k} - \langle a_{i_k}, x^K \rangle}{\|a_i\|^2} a_{i_k}$ 5: 6: 7: 8: 9: else $V_{k} = \max(0, X_{k})$ end if updates 10: $\sigma_k = \frac{1}{k+1}$ (change to $\sigma_k = \frac{1}{msweeps+1}$??) $x^{k+1} \leftarrow \sigma_k v + (1 - \sigma_k) v^k$ 11: 12: stopcrit $\leftarrow ||Av_0 - b||/(1 + ||b||)$ 13: $k \leftarrow k+1$ 14: if k mod (m+1) == 0 then 15: msweeps = msweeps + 116: 17: end if $i_k = k \pmod{m} + 1$ 18: end while

Numerical Tests varying sizes *m*, *n*

Table: Varying *m* = 100, 600, 1100, 1600

	Specifica	tions			Time (s)					Rel. Resid
	п	% density	Exact	Inexact	HLWB	LSQ	QPPAL	Exact	Inexact	HLWB
0	3000	8.1e-01	2.13e-03	1.98e-02	1.89e+01	3.22e+00	8.04e-01	2.55e-16	2.41e-15	2.29e-04
0	3000	8.1e-01	8.35e-02	3.03e-01	1.94e+02	4.28e+00	1.27e+00	5.10e-16	5.10e-18	2.19e-04
0	3000	8.1e-01	7.02e-01	1.29e+00	4.16e+02	6.18e+00	2.53e+00	5.20e-16	8.71e-16	2.08e-04
0	3000	8.1e-01	1.40e+00	3.59e+00	6.57e+02	7.65e+00	5.13e+00	9.84e-18	1.11e-15	2.27e-04

Table: Varying n, m = 200

	Specifica	ations			Time (s)					Rel. Resids.
	п	% density	Exact	Inexact	HLWB	LSQ	QPPAL	Exact	Inexact	HLWB
	3000	8.1e-01	3.12e-03	3.69e-02	4.45e+01	3.50e+00	8.66e-01	8.64e-18	7.39e-17	2.56e-04
	3500	8.1e-01	3.08e-03	4.05e-02	5.17e+01	4.93e+00	1.00e+00	9.07e-18	1.26e-17	2.78e-04
1	4000	8.1e-01	3.24e-03	3.70e-02	5.82e+01	7.31e+00	1.09e+00	1.46e-16	8.91e-16	2.80e-04
	4500	8.1e-01	3.99e-03	4.17e-02	6.58e+01	1.01e+01	1.18e+00	1.80e-15	2.05e-16	3.13e-04
	5000	8.1e-01	3.93e-03	3.42e-02	7.30e+01	1.45e+01	1.26e+00	4.09e-17	1.80e-15	3.16e-04

Table: Varying problem density, m = 300

Specifications				Time (s)					Rel. Resids.	
	'n	% density	Exact	Inexact	HLWB	LSQ	QPPAL	Exact	Inexact	HLWB
)	1000	1.0e+00	5.65e-03	5.69e-02	1.67e+01	3.02e-01	5.32e-01	7.48e-16	7.27e-16	1.54e-04
)	1000	6.0e+00	4.80e-02	2.52e-01	4.58e+01	3.15e-01	1.22e+00	3.44e-17	1.18e-16	1.51e-04
)	1000	1.1e+01	6.18e-02	2.49e-01	5.41e+01	3.07e-01	2.10e+00	5.65e-17	1.54e-17	1.44e-04
)	1000	1.6e+01	7.79e-02	2.60e-01	5.34e+01	3.03e-01	2.11e+01	6.92e-17	7.98e-17	1.61e-04

Solving (maximization) Linear Programs

primal (maximization) LP in standard form

$$\begin{array}{rcl} & \boldsymbol{p}_{LP}^* := & \max & \boldsymbol{c}^T \boldsymbol{x} \\ (\mathsf{PLP}) & & \mathsf{s.t.} & \boldsymbol{A} \boldsymbol{x} = \boldsymbol{b} \in \mathbb{R}^m \\ & & \boldsymbol{x} \in \mathbb{R}_+^n. \end{array}$$

dual LP

(DLP)
$$d_{LP}^* := \min_{\substack{b \in \mathcal{D}^T \\ s.t. \\ z \in \mathbb{R}^n_+}} b^T y$$
 (2)

Assumptions

A full row rank; $p^*_{LP} \in \mathbb{R}$ (so $p^*_{LP} = d^*_{LP} \in \mathbb{R}$ and both attained)

Geometric Algorithm

solution can be found from the limit as $R \uparrow \infty$ of the projection of the vector $v_R = Rc \in \mathbb{R}^n$ onto the feasible set.

Lemma ([20, 21, 22, 30])

Let the given LP data be A, b, c with finite optimal value p_{LP}^* . For each R > 0 define

$$egin{array}{rll} x(R) := & {
m argmin}_{x} & rac{1}{2} \|x - Rc\|^{2} \ s.t. & Ax = b \in \mathbb{R}^{m} \ x \in \mathbb{R}^{n}_{+}. \end{array}$$

Then x^* is the minimum norm solution of (PLP) if, and only if, there exists $\overline{R} > 0$ such that

$$R \geq \bar{R} \implies x^* \in \operatorname{argmin} \left\{ rac{1}{2} \|x - Rc\|^2 \, : \, Ax = b, \, x \in \mathbb{R}^n_+
ight\}$$

Avoid numerical/roundoff from large numbers

Corollary (scaling $\frac{1}{R}b$)

A, b, c, R, x(R) as in Lemma. Then

$$\begin{array}{rl} \frac{1}{R}x(R) = w(R) := & \operatorname{argmin}_{w} & \frac{1}{2} \|w - c\|^{2} \\ & s.t. & Aw = \frac{1}{R}b \in \mathbb{R}^{m} \\ & w \in \mathbb{R}^{n}_{+}. \end{array}$$

Proof.

From

$$||x - Rc||^{2} = R^{2} \left\| \frac{1}{R}x - c \right\|^{2} = R^{2} ||w - c||^{2}, x = Rw,$$

we substitute for x and obtain $A(Rw) = b \iff Aw = \frac{1}{R}b$. The result follows from the observation that argmin does not change after discarding the constant R^2 .

- efficient, robust algorithm for projection of a point onto a polyhedral set.
- One of may applications is to solving linear programs a type of exterior path following algorithm.

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Thanks for your attention!

Regularized Nonsmooth Newton Algorithms for Best Approximation with Applications



Tues. Mar. 28, 10:00-11:20 EST, 2023

joint work with: Yair Censor (Univ. of Haifa); Walaa Moursi and Tyler Weames (Univ. of Waterloo)