Interior-point method for nonlinear nonconvex optimization

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Outline

1. Introduction
2. Direction determination
3. Trust-region subproblem
4. Step-length selection
5. Numerical experiments

Outline

General nonlinear programming problem

Consider the general nonlinear programming problem

$$(\mathrm{NP}) \qquad x = \arg\min_{x \in \mathcal{R}^n} f(x) \quad \text{s.t.} \quad c_I(x) \le 0, \quad c_E(x) = 0,$$

where

$$c_I(x) = [c_i(x) : i \in I]^T, \qquad I = \{1, \dots, m_I\}$$
$$c_E(x) = [c_i(x) : i \in E]^T, \qquad E = \{m_I + 1, \dots, m_I + m_E = m\}.$$

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We assume that the functions

$$f(x) : \mathcal{R}^n \to \mathcal{R}, \quad c_I(x) : \mathcal{R}^n \to \mathcal{R}^{m_I}, \quad c_E(x) : \mathcal{R}^n \to \mathcal{R}^{m_E}$$

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are twice continuously differentiable.

Difficulty

This problem is hard to solve due to the presence of inequality constraints.

We introduce a slack vector

$$s \equiv s_I = [s_i(x) : i \in I]^T$$

and transform original problem (NP) to the sequence of problems with the logarithmic barrier function

$$\text{(IP)} \qquad x = \arg \min_{(x,s_I) \in \mathcal{R}^{n+m_I}} \left(F(x,s) \equiv f(x) - \mu e^T \ln(S_I) e \right)$$

subject to

$$c(x,s) \equiv [c_I(x) + s_I,\ c_E(x)] = 0$$

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where

- $\mu > 0$ is a barrier parameter, $\mu \to 0$ is assumed
- e is the vector with unit elements
- $S_I = \mathrm{diag}(s_i : i \in I)$

Let

$$\begin{aligned} \mathcal{L}(x, s, u_I, u_E) &= F(x, s) + u^T c(x, s) \\ &= f(x) - \mu e^T \ln(S_I) e + u_I^T (c_I(x) + s_I) + u_E^T c_E(x) \end{aligned}$$

be a Lagrange function of (IP) with Lagrange multipliers $u = [u_I, u_E]$. Then the necessary KKT conditions for the solution of problem (IP) have the following form (primal-dual formulation):

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$$\begin{aligned}\partial\mathcal{L}/\partial x &= g(x,u) = 0, \\ \partial\mathcal{L}/\partial s &= S_I U_I e - \mu e = 0, \\ \partial\mathcal{L}/\partial u_I &= c_I(x) + s_I = 0, \\ \partial\mathcal{L}/\partial u_E &= c_E(x) = 0,\end{aligned} \tag{1}$$

where

$$g(x,u) = \nabla f(x) + A_I(x)u_I + A_E(x)u_E,$$

$$A_I(x) = [\nabla c_i(x) : i \in I], \qquad A_E(x) = [\nabla c_i(x) : i \in E],$$

$$S_I = \mathrm{diag}(s_i : i \in I) \succ 0, \qquad U_I = \mathrm{diag}(u_i : i \in I) \succ 0.$$

Linearizing the primal-dual equations, we get one step of the Newton method

$$\begin{bmatrix} G_x & 0 & A_I & A_E \\ 0 & U_I & S_I & 0 \\ A_I^T & I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} d_x \\ d_s \\ d_{u_I} \\ d_{u_E} \end{bmatrix} = - \begin{bmatrix} g_x \\ S_I U_I e - \mu e \\ c_I + s_I \\ c_E \end{bmatrix}, \qquad (2)$$

where $d_x, d_s, d_{u_I}, d_{u_E}$ are direction vectors and

$$g_x = g(x,u) = \nabla f(x) + A_I(x) u_I + A_E(x) u_E$$

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- The Hessian matrix $G(x,u)$ is not usually given analytically, but automatic or numerical differentiation is used instead.
- We assume that the matrix of system (2) is nonsingular.

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2. Determine direction vectors $d_x, d_s, d_{u_I}, d_{u_E}$ satisfying (2).

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4. Set new iterations

$$x := x + \alpha d_x, \quad s_I := s_I(\alpha, d_s) > 0,$$

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5. Termination is when the KKT conditions are fulfiled.

Outline

Active and inactive constraints

KKT condition (1) implies that $S_I U_I e \approx \mu e$ and if $\mu \rightarrow 0$, then either $u_i \rightarrow 0$ or $s_i \rightarrow 0$ holds for every index $i \in I$. We split the set of inequality constraints to an active and inactive subsets.

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Active constraints

Are those for which $c_i(x)$, $i \in I$, are close to zero:

- $s_i \le \varepsilon_I u_i$, $i \in I$,
- they are denoted by $\hat{.}$, i.e. $\hat{c}_I(x), \hat{s}_I, \hat{u}_I$, where $\hat{c}_I \in \mathcal{R}^{\hat{m}_I}$.

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Inactive constraints

Are those for which u_i, $i \in I$, are close to zero:

- $s_i > \varepsilon_I u_i$, $i \in I$,
- they are denoted by $\check{.}$, i.e. $\check{c}_I(x), \check{s}_I, \check{u}_I$, where $\check{u}_I \in \mathcal{R}^{\check{m}_I}$.

Here $\varepsilon_I > 0$ is a suitable parameter and $\hat{m}_I + \check{m}_I = m_I$.

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original system (2)

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where

$$\begin{aligned} D_I &= (S_I U_I^{-1})^{1/2} \\ D_I g_s &= (S_I U_I)^{1/2} e - \mu (S_I U_I)^{-1/2} e \end{aligned}$$

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Disadvantage

Elements of matrix $S_I U_I^{-1}$ can be unbounded since $u_i \to 0$ if the i-th inequality constraint is inactive at the solution point.

Inactive equations are eliminated and computed directly afterwards

$$\begin{aligned} \check{d}_s &= -(\check{c}_I + \check{A}_I^T d_x + \check{s}_I) \\ \check{d}_{u_I} &= \check{S}_I^{-1} \check{U}_I (\check{c}_I + \check{A}_I^T d_x) + \mu \check{S}_I^{-1} e \end{aligned}$$

while active parts are computed iteratively from the system

$$\begin{bmatrix} \hat{G}_x & 0 & \hat{A}_I & A_E \\ 0 & I & \hat{D}_I & 0 \\ \hat{A}_I^T & \hat{D}_I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} d_x \\ \hat{D}_I^{-1} \hat{d}_s \\ \hat{d}_{u_I} \\ d_{u_E} \end{bmatrix} = - \begin{bmatrix} \hat{g}_x \\ \hat{D}_I \hat{g}_s \\ \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix}, \qquad (3)$$

where

$$\hat{D}_I = (\hat{S}_I \hat{U}_I^{-1})^{1/2}, \quad \hat{D}_I \hat{g}_s = (\hat{S}_I \hat{U}_I)^{1/2} e - \mu (\hat{S}_I \hat{U}_I)^{-1/2} e,$$

$$\hat{G}_x = G_x + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{A}_I^T, \quad \hat{g}_x = g_x + \check{A}_I \check{S}_I^{-1} \check{U}_I \check{c}_I + \mu \check{A}_I \check{S}_I^{-1} e.$$

Matrices $\hat{S}_I \hat{U}_I^{-1}$ and $\hat{G}_x$ and vector $\hat{g}_x$ are bounded (if original G_x, g_x, and $[A_I, A_E]$ are bounded) and if the strict complementarity conditions

$$\lim_{\mu \to 0} (s_i + u_i) > 0, \quad i \in I,$$

hold (recall that $s_i > 0$, $u_i > 0$ and $s_i \to 0$ or $u_i \to 0$), then

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$$\lim_{\mu \to 0} \hat{S}_I \hat{U}_I^{-1} = 0.$$

Similarly, the matrix $\check{S}_I^{-1} \check{U}_I$ is bounded and if the strict complementarity conditions hold, then

$$\lim_{\mu \to 0} \check{S}_I^{-1} \check{U}_I = 0.$$

Direction determination - summary

Simplified form of (3):

$$\begin{bmatrix} \hat{G}_x & 0 & \hat{A}_I & A_E \\ 0 & I & \hat{D}_I & 0 \\ \hat{A}_I^T & \hat{D}_I & 0 & 0 \\ A_E^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} d_x \\ \hat{D}_I^{-1} \hat{d}_s \\ \hat{d}_{u_I} \\ d_{u_E} \end{bmatrix} = - \begin{bmatrix} \hat{g}_x \\ \hat{D}_I \hat{g}_s \\ \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix}$$

$\Leftrightarrow$

$$\begin{bmatrix} B & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d \\ d_u \end{bmatrix} = - \begin{bmatrix} g \\ h \end{bmatrix} \tag{4}$$

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where

$$B = \begin{bmatrix} \hat{G}_x & 0 \\ 0 & I \end{bmatrix}, \quad A = \begin{bmatrix} \hat{A}_I & A_E \\ \hat{D}_I & 0 \end{bmatrix}, \quad g = \begin{bmatrix} \hat{g} \\ \hat{D}_I \hat{g}_s \end{bmatrix}, \quad h = \begin{bmatrix} \hat{c}_I + \hat{s}_I \\ c_E \end{bmatrix},$$

$$d = \begin{bmatrix} d_x \\ \hat{D}_I^{-1}\hat{d}_s \end{bmatrix}, \quad d_u = \begin{bmatrix} \hat{d}_{u_I} \\ d_{u_E} \end{bmatrix}$$

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- Inactive directions $\check{d}_s, \check{d}_{u_I}$ are computed directly afterwards

Outline

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have exactly form (4).

- We can use a trust region method to (5) with a constraint

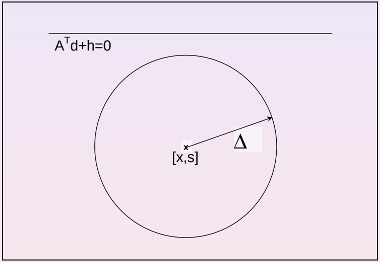
$$\|d\| \leq \Delta$$

to obtain a direction vector d.

As both constraints

$$A^T d + h = 0, \quad \|d\| \le \Delta$$

can be incompatible,



we will use the idea of Byrd and Omojokun, to make both constraints compatible and secure a sufficient decrease of $Q(d)$:

$$d = d_V + d_H$$

First, consider the problem

$$\min \; \|A^T d + h\| \quad \text{s.t.} \quad \|d\| \le \delta\Delta$$

for $0 < \delta < 1$ (e.g. $\delta = 0.8$).

Vertical subproblem

This problem is equivalent to

$$\min \; Q_V(d) = \frac{1}{2} d^T A A^T d + h^T A^T d \quad \text{s.t.} \quad \|d\| \le \delta\Delta$$

We suppose that A has a full column rank.

We compute the Cauchy and the Newton steps

$$d_C = -\frac{\|Ah\|^2}{\|A^T Ah\|^2} Ah, \qquad d_N = -A(A^T A)^{-1} h$$

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- if $\|d_C\| \ge \delta\Delta$, then set

$$d_V = \frac{\delta\Delta}{\|d_C\|} d_C$$

The Dennis-Mei dogleg method

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$$d_V = \frac{\delta\Delta}{\|d_C\|} d_C$$

- if $\|d_N\| \le \delta\Delta$, then set

$$d_V = d_N$$

We compute the Cauchy and the Newton steps

$$d_C = -\frac{\|Ah\|^2}{\|A^T Ah\|^2} Ah, \qquad d_N = -A(A^T A)^{-1} h$$

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- in the remaining case $\|d_C\| < \delta\Delta < \|d_N\|$, set

$$d_V = d_C + \kappa(d_N - d_C),$$

where $\kappa > 0$ is chosen so that $\|d_V\| = \delta\Delta$

Horizontal subproblem I.

Reformulation of original subproblem (5):

$$\min \;\; Q_H(d) = 1/2\, d^T B d + g^T d \quad \text{s.t.} \quad \|d\| \le \Delta, \quad A^T d = A^T d_V$$

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The constraints are compatible ($d = d_V$ satisfies them) and since we require $d = d_V + d_H$, for a solution d_H it follows that

$$A^T d_H = 0, \quad d_H = Z d_Z, \quad d_V^T d_H = 0$$

where the columns of Z form a basis of the null space of A^T.

Horizontal step

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Horizontal subproblem II.

Substitution into Q_H leads to a subproblem for d_Z

$$\min \ Q_Z(d) = 1/2\, d^T B_Z d + g_Z^T d \quad \text{s.t.} \quad \|Zd\| \le \Delta_Z$$

$$B_Z = Z^T B Z, \quad g_Z = Z^T (B d_V + g), \quad \Delta_Z = \sqrt{\Delta^2 - \|d_V\|^2}$$

The Steihaug-Toint conjugate gradient method

- We use the preconditioned conjugate gradient method with the preconditioner

$$C = Z^T Z$$

and include these iterations in original subproblem (5) for $d = d_V + Zd_Z$ with $\|d\| \le \Delta$.

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- The use of $d_H = Zd_Z$ leads to multiplication by the matrix

$$P_Z = Z(Z^T Z)^{-1} Z^T \equiv I - A(A^T A)^{-1} A^T = P_A$$

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- Lagrange multipliers d_u cannot be computed from the CG method. From (4) we have

$$Ad_u = -(g + Bd) \equiv -r$$

where r is a residuum. Thus

$$d_u = -(A^T A)^{-1} A^T r$$

as a solution of a least squares problem.

The algorithm

Iterations for original subproblem (5) have the form

1. $d = d_V, \quad r = Bd + g, \quad d_u = -(A^T A)^{-1} A^T r,$
   $\tilde{r} = r + A d_u, \quad p = -\tilde{r}$
2. $\eta = p^T B p, \quad \alpha = \frac{r^T \tilde{r}}{\eta}, \quad d^+ = d + \alpha p$
3. $r^+ = r + \alpha B d, \quad d_u^+ = -(A^T A)^{-1} A^T r^+,$
   $\tilde{r}^+ = r^+ + A d_u^+, \quad \beta = \frac{{r^+}^T \tilde{r}^+}{r^T \tilde{r}}, \quad p^+ = -\tilde{r}^+ + \beta p$

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Termination

negative curvature is encountered if $\eta \le 0$ then $d_\star = d + \kappa p$,

where $\kappa > 0$ is chosen so that $\|d_\star\| = \Delta$;

$r_\star = r + \kappa B p, \; d_{u\star} = -(A^T A)^{-1} A^T r_\star$

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unconstrained solution with sufficient precision if $\|r^+\| \le \varepsilon \|g\|$,
then $d_\star = d^+$, $d_{u\star} = d_u^+$

Outline

Back to the original problem:

$$x = \arg \min_{(x,s_I)\in\mathcal{R}^{n+m_I}} \left(F(x,s) \equiv f(x) - \mu e^T \ln(S_I)e \right)$$

subject to

$$c(x,s) \equiv [c_I(x) + s_I,\ c_E(x)] = 0$$

with Lagrange multipliers

$$u = [u_I, u_E]$$

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After determination of active components $d_x, \hat{d}_s, \hat{d}_{u_I}, d_{u_E}$ from the Byrd-Omojokun trust-region subproblem we compute inactive components $\check{d}_s, \check{d}_{u_I}$ to obtain the quantities d_s, d_{u_I}.

New iteration step

Now we define

$$x^+ = x + \alpha_x d_x, \quad s_I^+ = s_I + \alpha_s d_s,$$

$$u_I^+ = u_I + \alpha_{u_I} d_{u_I}, \quad u_E^+ = u_E + \alpha_{u_E} d_{u_E}$$

such that $s_I^+ > 0$ and $u_I^+ > 0$ hold using the bounds $\bar{\alpha}_s$ and $\bar{\alpha}_{u_I}$.

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such that $s_I^+ > 0$ and $u_I^+ > 0$ hold using the bounds $\bar{\alpha}_s$ and $\bar{\alpha}_{u_I}$.

Accepted step

The step x^+, s^+, u^+ is accepted if for $\alpha = 1$, where

$$\alpha_x = \alpha, \quad \alpha_s = \min(\alpha, \bar{\alpha}_s), \quad \alpha_{u_I} = \min(\alpha, \bar{\alpha}_{u_I}), \quad \alpha_{u_E} = \alpha$$

we have

$$F(x^+, s^+) < F(x, s) \quad \text{or} \quad \|c(x^+, s^+)\| < \|c(x, s)\|$$

Otherwise, the step is rejected ($\alpha_x = \alpha_s = \alpha_{u_I} = \alpha_{u_E} = 0$).

To decide if the step is acceptable, we define

- the merit function $P(\alpha)$ with the coefficient $\sigma > 0$:

$$\begin{aligned} P(\alpha) &= F(x + \alpha_x d_x, s + \alpha_s d_s) \\ &+ (u + d_u)^T c(x + \alpha_x d_x, s + \alpha_s d_s) \\ &+ \frac{\sigma}{2} \|c(x + \alpha_x d_x, s + \alpha_s d_s)\|^2 \end{aligned}$$

The merit function

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- and its quadratic approximation

$$Q(\alpha) = P(0) + \alpha P'(0) + \frac{\alpha^2}{2} d^T B d$$

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$$Q(\alpha) = P(0) + \alpha P'(0) + \frac{\alpha^2}{2} d^T B d$$

We can use another merit function but $P(\alpha)$ has shown to be the best in practical computations.

Actual decrease: defined as $P(1) - P(0)$

Predicted decrease: defined as $Q(1) - Q(0)$

Feasible step

Theorem

The condition

$$Q(1) - Q(0) < 0$$

is necessary for applying the trust-region method. It holds provided

$$\sigma > \frac{\frac{1}{2}d^T B d + d^T g + d^T A d_u}{-d^T A c}$$

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Now we can define the number

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The step is

:-) accepted if $\varrho > 0$: k-th iteration $\rightsquigarrow$ $(k+1)$-st iteration

:-(rejected if $\varrho \leq 0$: choose $\Delta < \|d\|$ and compute new direction vectors in the k-th iteration

- Update of Δ:

$$
\begin{aligned}
\Delta^+ &= \beta\|d\| < \Delta && \text{if} \quad \varrho < \underline{\varrho} \\
\Delta^+ &= \Delta && \text{if} \quad \underline{\varrho} \le \varrho \le \overline{\varrho} \\
\Delta^+ &= \gamma\Delta > \Delta && \text{if} \quad \overline{\varrho} < \varrho
\end{aligned}
$$

Here $0 < \beta < 1 < \gamma$ and $0 < \underline{\varrho} < \overline{\varrho} < 1$.

Update of parameters

- Update of Δ:

$$\begin{aligned} \Delta^+ &= \beta\|d\| < \Delta & \text{if} \quad & \varrho < \underline{\varrho} \\ \Delta^+ &= \Delta & \text{if} \quad & \underline{\varrho} \le \varrho \le \overline{\varrho} \\ \Delta^+ &= \gamma\Delta > \Delta & \text{if} \quad & \overline{\varrho} < \varrho \end{aligned}$$

  Here $0 < \beta < 1 < \gamma$ and $0 < \underline{\varrho} < \overline{\varrho} < 1$.

- Barrier parameter μ is changed each iteration by a heuristic approach:

$$\mu = \nu \frac{s^T u_I}{m_I}$$

  where

$$\nu = \frac{1}{10} \min\left\{\frac{1-\omega}{20\omega}, 2\right\}^3 \quad \text{and} \quad \omega = \frac{\min_{i\in I}\{s_i u_i\}}{s^T u_I / m_I}$$

Outline

The methods for constrained optimization are implemented in the interactive system for universal functional optimization UFO

www.cs.cas.cz/luksan/ufo.html

[1] [L,M,V: Interior point method for non-linear non-convex optimization, NLAA, 2004(11), 431-454]

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IPCGM indefinitely preconditioned conj. gradient method [1] applying to system (4)

$$\begin{bmatrix} B & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d \\ d_u \end{bmatrix} = - \begin{bmatrix} g \\ h \end{bmatrix}$$

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We have performed numerical comparison of methods for direction determination

- IPCGM indefinitely preconditioned conj. gradient method [1] applying to system (4)
- TRM trust-region method applying to subproblem (5)

$$\min \;\; Q(d) = \frac{1}{2} d^T B d + g^T d \quad \text{s.t.} \quad A^T d + h = 0$$

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All problems have the dimension $n = 1000$.

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Columns of tables

- `Constr.` are the constraints used,
- `Method` is the method for the direction determination used,
- `NIT` is the total number of iterations,
- `NFV` is the total number of function evaluations,
- `NFG` is the total number of gradient evaluations,
- `NF` is the total number of failures,
- `NT` is the total number of tuned parameters,
- `NB` is the total number of better computed examples,
- `Time` is the total computational time in seconds.

Comparison

Constr.	Method	NIT	NFV	NFG	NF	NT	NB	Time
$c(x) \geq 0$	IPCGM	695	931	4989	0	7	0	4.67
	TRM	1385	1528	11575	0	10	5	5.94
$c(x) \leq 0$	IPCGM	2196	3147	14023	0	3	2	13.20
	TRM	1798	1872	11782	2	3	0	9.24
$x \geq 0$,	IPCGM	811	1386	6597	0	5	0	6.89
$c(x) \geq 0$	TRM	1255	1378	9073	0	5	1	5.74
$x \leq 0$,	IPCGM	562	833	4149	1	1	1	6.77
$c(x) \leq 0$	TRM	759	828	5501	2	4	0	7.11
$\|x\| \leq 1$,	IPCGM	613	825	4637	0	4	1	4.31
$\|c(x)\| \leq 1$	TRM	1182	1297	8124	1	6	3	9.38

Conclusion

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- Better procedures must be developed to overcome problems with incompatibility of constraints.
- A very important part is a suitable choice of the merit function to decide if the step is feasible (new approaches: filter technique, trust-funnel algorithm).

Thank you for your attention!