Algorithms for Solving MINLPs under Partial and Non-differentiability Assumptions

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Outline

Why Derivative-free Methods?

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2. Pattern Search: Converges but only if $f(x)$ is Differentiable
3. Model based Methods: Good Algorithms have been Developed for Bound or Linear Constraints but no Theoretical Convergence

Many Problem are Solved Anyway But Good Accuracies either not Possible or bring Burden to Function Evaluations

We Consider Mixed Integer Program

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$$(MP)\begin{cases} \min\limits_{x_c, x_d} \; f(x_c, x_d) \\ s.t. \;\; g_i(x_c, x_d) \leq 0, i = 1, \cdots, m, \\ \qquad x_c \in X, x_d \in Y \; integer, \end{cases} \tag{2}$$

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- $Y \subset \mathbb{R}^p$ is a polyhedral set of integers

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Combined?

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4. The Inner Radius ρ_k is used to Restrict the Placement of new Interpolation Points, Stopping BOBYQA.

$$
\begin{aligned}
\min_{d_k} \quad & Q_k(x_k + d_k) \\
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& \|d_k^T\| \leq \Delta_k
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$$\begin{aligned} \max_{d_k} \quad & |\Lambda_t(x_k + d_k)| \\ \text{s.t.} \quad & l \leq x_k + d_k \leq u, \\ & \|d_k^T\| \leq \Delta_k \end{aligned} \tag{5}$$

$$Q_k(y_i) = f(y_i), \quad i \in K, \tag{6}$$

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$$x_{k+1} = \begin{cases} x_k, & f(x_k) \leq f(x_k + d_k), \\ x_k + d_k, & f(x_k) > f(x_k + d_k). \end{cases}$$

$$Q_{k+1}(\widehat{y}_i) = f(\widehat{y}_i), \quad i \in K. \tag{8}$$

Generate Q_{k+1} **from** Q_k **by minimising** $\|\nabla^2 Q_{k+1} - \nabla^2 Q_k\|_F$ **subject to**

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This is Done by Solving a System of Linear Equations.

$$\left[\begin{array}{c|c} A & Y^T \\ \hline Y & 0 \end{array}\right] \left[\begin{array}{c} \lambda \\ \hline p \\ q \end{array}\right] = \left[\begin{array}{c} r \\ \hline 0 \end{array}\right],$$

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$$W = \left[\begin{array}{c|c} A & Y^T \\ \hline Y & 0 \end{array}\right]^{-1} = \left[\begin{array}{c|c} \Omega & \Xi^T \\ \hline \Xi & 0 \end{array}\right].$$

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4. Constraints in the Subproblem: Quadratic to Linear

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These MIQPs are Solved basing on H_{cc} being PD, PSD, Indefinite

Definition

(Continuous local minimum) A point $x^* \in \Omega_c$ is a local minimum if, for some $\epsilon > 0$,

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(Global minimum) A point $x^* \in \Omega_m$ is a global minimum if,

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i) A point is a local minimum of a continuous, convex problem if and only if it is the global minimum.

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ii) If $n_c = 0$ (discrete problem) and $\mathcal{N}_d(x) = \Omega_d$ then a point is a local minimum of the problem if and only if it is a global minimum.

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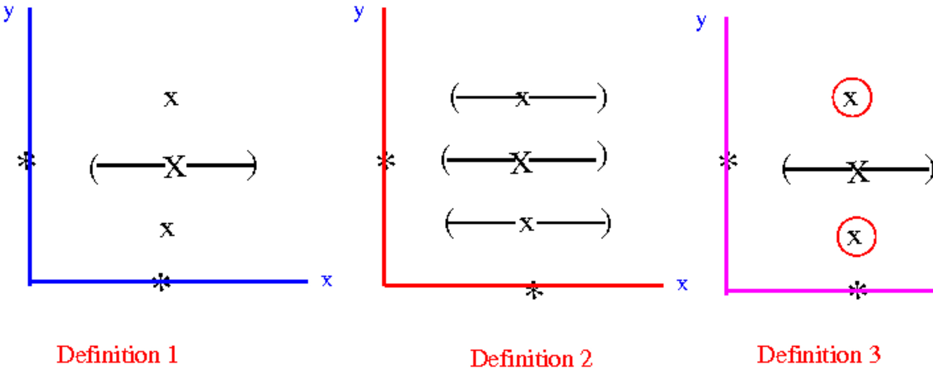
4) If $\mathcal{N}_m$ contains at least one point on each *feasible continuous manifold* and f and c_i are convex then a point is a local minimum of a mixed integer problem if and only if it is a global minimum.

Figure: Definition of the New Local Minimum



Definition

(Separate local minimum) A point $x^* \in \Omega_m$ is a local minimum if, for some $\epsilon > 0$,

$$f(x^*) \leq f(x), \quad \forall x \in \{x : x_c \in B_\varepsilon(x_c^*),\ x_d = x_d^*\} \cap \Omega_m, \tag{12}$$

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$$\mathcal{N}_r(x) = \{y \in \mathbb{R}^n : y_c = x_c,\ \|y_d - x_d\| \le 1\}.$$

Definition

(Combined local minimum) A point $x^* \in \Omega_m$ is a local minimum if, for some $\epsilon > 0$,

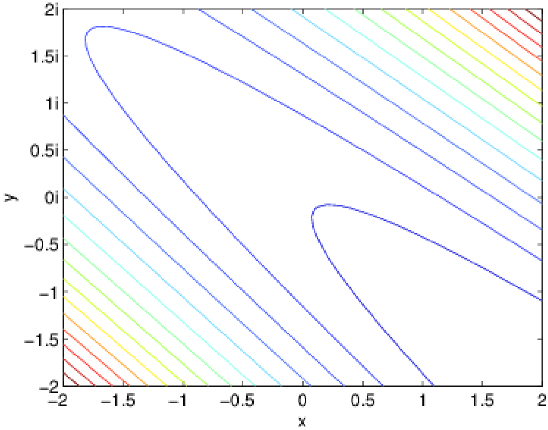
$$f(x^*) \leq f(x), \quad \forall x \in \{x : x_c \in B_\varepsilon(x_c^*),\, x_d = x_d^*\} \cap \Omega_m, \tag{14}$$

$$f(x^*) \leq f(x), \quad \forall x \in \mathcal{N}_{\text{comb}}(x^*) \cap \Omega_m. \tag{15}$$

where $\mathcal{N}_{\text{comb}}(x^*)$ is the set of smallest local minima on each *feasible continuous manifold* on which $\mathcal{N}_r(x^*)$ has a point.

$$\begin{aligned} \min_{[y,x]} \quad & \frac{5}{2}(x+y)^2 + \frac{1}{\sqrt{2}}(-x+y) \qquad (16) \\ \text{s.t.} \quad & -2 \le x, y \le 2, \\ & y \in \mathbb{R},\ x \in \mathbb{Z}. \end{aligned}$$

Figure: Definition of the New Local Minimum



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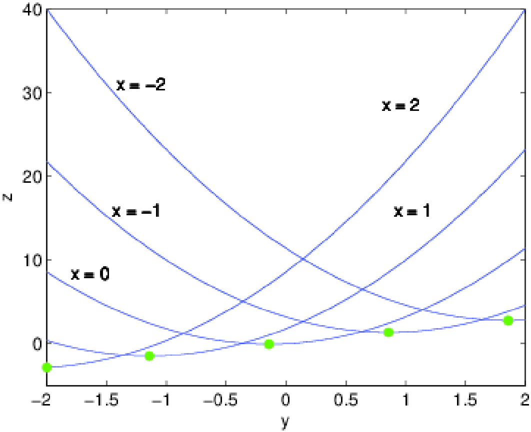

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Finite Convergence Proof within ε Neighborhood for SEMBOQA and COMBOQA

Newby & Ali (2014): Computational Optimization and Applications

Figure: Performance Profile using Function Values

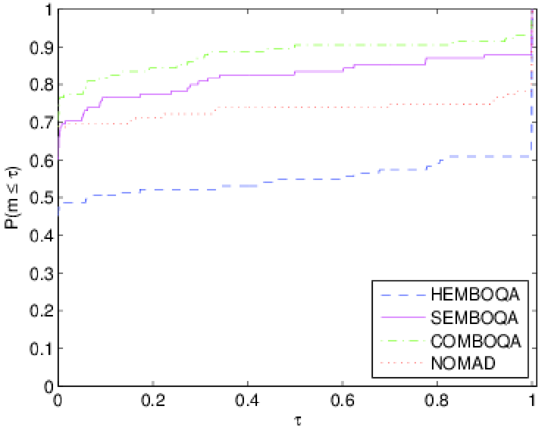
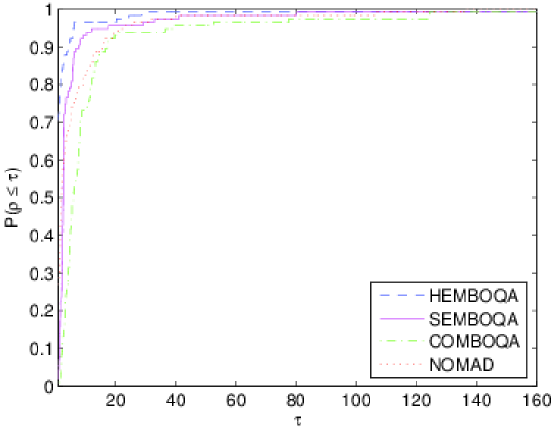


Figure: Performance Profile using CPU Times



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Outer Approximation for convex and Smooth MINLPs

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Key Idea: Reformulate MINLP as an MILP: (Duran and Grossmann, 1986; Fletcher and Leyffer, 1994)

Given some set K with optimal solutions of NLP subproblems, build a relaxation of (MP):

$$
\left\{
\begin{array}{ll}
\min \ \theta & \\
s.t. \ f(x_j, y_j) + \nabla f(x_j, y_j)^T \begin{pmatrix} x - x_j \\ y - y_j \end{pmatrix} \le \theta, & \\
\qquad g_i(x_j, y_j) + \nabla g_i(x_j, y_j)^T \begin{pmatrix} x - x_j \\ y - y_j \end{pmatrix} \le 0, \forall i, & \forall (x_j, y_j) \in K \\
\qquad x \in X, y \in Y \ \ integer &
\end{array}
\right.
$$

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f, g_i are Convex, but not Differentiable

Convex MINLP with Non-differentiable Data

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$$\begin{cases} \min\limits_{x,y} \quad f(x,y) = x_2 \\ s.t. \quad g(x,y) = x_1^2 + x_2^2 + |y| - 2 \leq 0, \\ \; x = (x_1, x_2) \in \mathbb{R}^2, \; y \in \{-1, 0, 1, 3\} \end{cases}$$

Theorem

Let $\phi : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}$ be continuous convex function and $(\bar{x}, \bar{y}) \in \mathbb{R}^n \times \mathbb{R}^p$. Then for any $\bar{\alpha} \in \partial\phi(\cdot, \bar{y})(\bar{x})$, there exist $\bar{\beta} \in \mathbb{R}^p$ such that $(\bar{\alpha}, \bar{\beta}) \in \partial\phi(\bar{x}, \bar{y})$.

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Divide Y into two sets:

$$\begin{cases} T := \{y_j \in Y : P(y_j) \textit{ is feasible}\} \\ S := \{y_l \in Y : P(y_l) \textit{ is infeasible}\} \end{cases}$$

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$$0 \in \partial f(\cdot, y_j)(x_j) + \sum_{i=1}^{m} \lambda_{j,i} \partial g_i(\cdot, y_j)(x_j) + N(X, x_j)$$

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Take $\alpha_j \in \partial f(\cdot, y_j)(x_j)$ and $\xi_{j,i} \in \partial g_i(\cdot, y_j)(x_j)(i = 1, \cdots, m)$.

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It is proved that there exist β_j and $\eta_{j,i}$ such that

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Substitute gradients with subgradients:

$$\nabla f(x_j, y_j) \leftarrow (\alpha_j, \beta_j)$$
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\min\limits_{x,y,\theta} \quad \theta \\
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However, this Procedure may be not Valid if arbitrary Subgradients are chosen to Replace Gradients. See the following example:

$$\begin{cases} \min\limits_{x,y} & f(x,y) := x + y \\ s.t. & g_1(x,y) := \max\{-x+y+1, x-y+1\} \leq 0, \\ & g_2(x,y) := x - y \leq 0, \\ & x \in [0,2],\ \ y \in \{1,2,3\}. \end{cases}$$

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Since KKT conditions at (x_0, y_0) for $(\xi_{0,1}, \eta_{0,1})$ does not hold:

$$\nexists (\lambda_{0,1}, \lambda_{0,2}) \in \mathbb{R}^2_+ \ \textit{with} \ \nabla f(x_0, y_0) + \lambda_{0,1}(\xi_{0,1}, \eta_{0,1}) + \lambda_{0,2} \nabla g_2(x_0, y_0) = 0.$$

Mixed-integer Nonlinear Programming Problem (MINLPs)

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$f : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}$, $g : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$ are nonlinear functions

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For MINLP (MP), take $E := \mathbb{R}^n$, $Z := \mathbb{R}^m$, $D := \mathbb{R}^p$ and $K := \mathbb{R}^m_+$

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$$D \quad \max_{u^* \in K^+} \left[\inf_{x \in X} \{ f(x) + \langle u^*, g(x) \rangle \} \right],$$

$K^+ := \{ z^* \in Z^* : \langle z^*, z \rangle \geq 0, \ \forall z \in K \}$ — the Dual Cone of K.

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Let $y \in Y$ be Fixed. Consider Primal Problem $P(y)$:

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Generalized Benders Decomposition for (VOP)

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RMP^{k,j}\left\{\begin{array}{ll}
\min\limits_{y,\eta} & \eta \\
s.t. & \inf\limits_{x\in X}\{f(x,y)+\langle u_{i,j}^{*}, g(x,y)\rangle\} \leq \eta, \quad \forall i=1,\cdots,k, \\
 & \inf\limits_{x\in X}\langle z_{k,l}^{*}, g(x,y)\rangle \leq 0, \quad \forall l=1,\cdots,j, \\
 & y\in Y, \eta\in\mathbb{R}.
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$$RMP^{k,j}\begin{cases}\min\limits_{y,\eta} & \eta\\ s.t. & \inf\limits_{x\in X}\{f(x,y)+\langle u^*_{i,j},g(x,y)\rangle\}\leq\eta,\quad\forall i=1,\cdots,k,\\ & \inf\limits_{x\in X}\langle z^*_{k,l},g(x,y)\rangle\leq 0,\quad\forall l=1,\cdots,j,\\ & y\in Y,\eta\in\mathbb{R}.\end{cases}$$

Denote $(y_{k+1,j},\eta_{k+1,j})$ optimal solution of $RMP^{k,j}$.

Generalized Benders Decomposition for (VOP)

$$
RMP^{k,j+1}\begin{cases}\min\limits_{y,\eta}\ \eta\\ s.t.\ \eta \geq \inf\limits_{x\in X}\{f(x,y)+\langle u_{i,j}^{*}, g(x,y)\rangle\},\quad \forall i=1,\cdots,k,\\ \qquad \inf\limits_{x\in X}\langle z_{k,l}^{*}, g(x,y)\rangle \leq 0,\quad \forall l=1,\cdots,j,j+1,\\ \qquad y\in Y,\ \eta\in\mathbb{R}.\end{cases}
$$

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$$RMP^{k,j+1}\begin{cases}\min\limits_{y,\eta} \ \eta \\ s.t. \ \eta \geq \inf\limits_{x\in X}\{f(x,y)+\langle u^*_{i,j}, g(x,y)\rangle\}, \quad \forall i=1,\cdots,k, \\ \qquad \inf\limits_{x\in X}\langle z^*_{k,l}, g(x,y)\rangle \leq 0, \quad \forall l=1,\cdots,j,j+1, \\ \qquad y\in Y,\ \eta\in\mathbb{R}.\end{cases}$$

Denote $(y_{k+1,j+1}, \eta_{k+1,j+1})$ the optimal solution of $RMP^{k,j+1}$.

Thank You!