Globally Convergent Optimization Methods Based on Conservative Convex Approximations

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Outline

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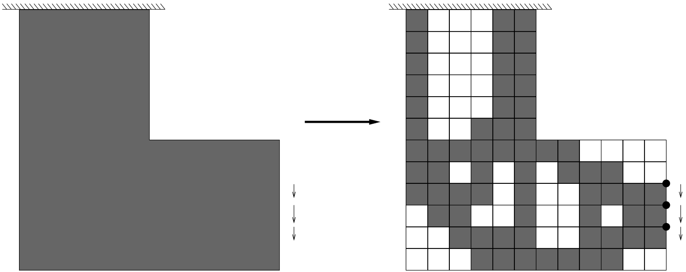
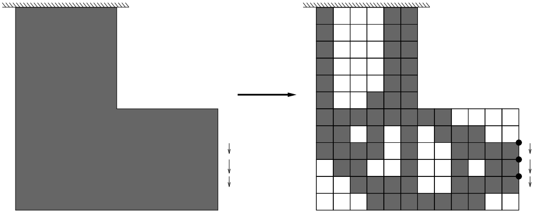
1. Application background
2. Conservative convex approximations – main ideas
3. Global convergence
4. Extended/restricted problem formulation

Ground structure approach for topology optimization



- The discretized structure has n finite elements.
- The design is represented by $\mathbf{x} \in \{0, 1\}^n$.
- Elements filled with material have $x_j = 1$ (black).
- Elements without material have $x_j = 0$ (white).

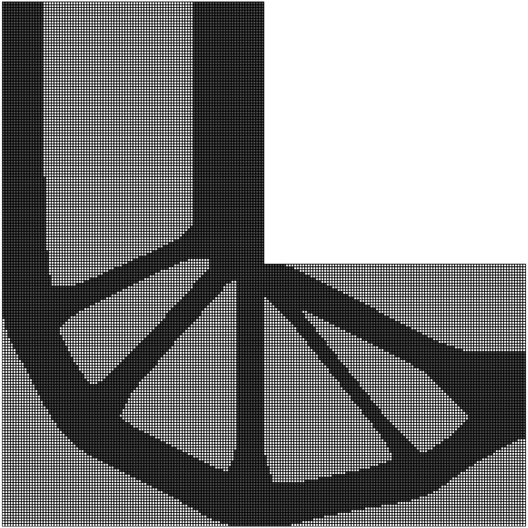
Possible topology optimization problem



- $\mathbf{f}$ = vector of (given) external nodal forces,
- $\mathbf{d}$ = vector of nodal displacements,
- $\mathbf{K}(\mathbf{x}) = \sum_{j=1}^{n} x_j \mathbf{K}_j$ = structural stiffness matrix.
- State equations: $\mathbf{K}(\mathbf{x})\mathbf{d} = \mathbf{f}$.

Possible problem: minimize $\sum_{j=1}^{n} x_j$ subject to $\mathbf{f}^{\mathsf{T}}\mathbf{d}(\mathbf{x}) \leq S$, where $\mathbf{d}(\mathbf{x})$ is a solution to the state equations.

Possible solution, 27648 variables



Naive but possible heuristic approach

Replace the integer programming problem by a relaxed and penalized continuous nonlinear programming problem

$$
\begin{aligned}
\text{minimize} \quad & \sum_{j=1}^{n} x_j \; + \; C \sum_{j=1}^{n} x_j(1-x_j)) \\
\text{subject to} \quad & \mathbf{f}^{\mathsf{T}}\mathbf{d}(\mathbf{x}) \leq S, \\
& 0 \leq x_j \leq 1, \quad j = 1, \ldots, n.
\end{aligned}
$$

where $\mathbf{d}(\mathbf{x})$ is the solution to $(\sum_{j=1}^{n} x_j \mathbf{K}_j)\mathbf{d} = \mathbf{f}$.

The penalty parameter C is gradually increased from zero, until (almost) all $x_j \in \{0, 1\}$.

Characteristics of topology optimization problems

Some typical properties of the (relaxed and penalized) nonlinear programming problems in topology optimization:

- Nonconvex problem with a large number of variables.
- Given lower and upper bounds on the variables.
- Relatively few general nonlinear constraints (inequalities).
- Expensive function evaluations...
- ...but still possible to calculate derivatives.
- Not always important with high accuracy optimality...
- ...but the algorithms should be reliable.

One frequently used solution method is the *method of moving asymptotes* (MMA), which is based on the concept of conservative convex approximations.

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Conservative convex approximations

Consider a problem of the following type:

$$\begin{aligned} \text{minimize} \quad & f_0(\mathbf{x}) \\ \text{subject to} \quad & f_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m, \end{aligned}$$

where $\mathbf{x} \in R^n$ and $f_0, f_1, \ldots, f_m$ are given continuously differentiable functions.

Approximating subproblem

At iteration k, the feasible iteration point $\mathbf{x}^{(k)} \in R^n$ is given.
A corresponding convex first order approximating subproblem is defined by

$$\begin{aligned} &\text{minimize} && \tilde{f}_0^{(k)}(\mathbf{x}) \\ &\text{subject to} && \tilde{f}_i^{(k)}(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m, \end{aligned}$$

where $\tilde{f}_0^{(k)}, \tilde{f}_1^{(k)}, \ldots, \tilde{f}_m^{(k)}$ are certain convex functions which satisfy $\tilde{f}_i^{(k)}(\mathbf{x}^{(k)}) = f_i(\mathbf{x}^{(k)})$ and $\nabla \tilde{f}_i^{(k)}(\mathbf{x}^{(k)}) = \nabla f_i(\mathbf{x}^{(k)})$.
In particular, $\tilde{f}_0^{(k)}$ should be strictly convex.

The optimal solution $\hat{\mathbf{x}}^{(k)}$ of this subproblem possibly becomes the next iteration point $\mathbf{x}^{(k+1)}$.

Linear + separable quadratic approximations

A simple example of a convex first order approximating subproblem is

$$\begin{aligned} \text{minimize} \quad & f_0(\mathbf{x}^{(k)}) + \nabla f_0(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_0^{(k)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2 \\ \text{subject to} \quad & f_i(\mathbf{x}^{(k)}) + \nabla f_i(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_i^{(k)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2 \leq 0, \\ & i = 1, \ldots, m, \end{aligned}$$

where $\rho_0^{(k)} > 0$ and $\rho_i^{(k)} \geq 0$ for $i = 1, \ldots, m$.

Easy to solve, e.g. by a dual method, due to the convexity and separability.

Conservative approximating subproblem

The convex first order approximating subproblem

$$\begin{aligned} \text{minimize} \quad & \tilde{f}_0^{(k)}(\mathbf{x}) \\ \text{subject to} \quad & \tilde{f}_i^{(k)}(\mathbf{x}) \leq 0, \quad i = 1, \dots, m, \end{aligned}$$

with optimal solution $\hat{\mathbf{x}}^{(k)}$, is a conservative approximating subproblem if $\tilde{f}_i^{(k)}(\hat{\mathbf{x}}^{(k)}) \geq f_i(\hat{\mathbf{x}}^{(k)})$ for $i = 0, 1, \dots, m$.

In that case,
$f_i(\hat{\mathbf{x}}^{(k)}) \leq \tilde{f}_i^{(k)}(\hat{\mathbf{x}}^{(k)}) \leq 0$, for $i = 1, \dots, m$,
$f_0(\hat{\mathbf{x}}^{(k)}) \leq \tilde{f}_0^{(k)}(\hat{\mathbf{x}}^{(k)}) < \tilde{f}_0^{(k)}(\mathbf{x}^{(k)}) = f_0(\mathbf{x}^{(k)})$, unless $\hat{\mathbf{x}}^{(k)} = \mathbf{x}^{(k)}$.

Reasonable to let $\hat{\mathbf{x}}^{(k)}$ become the next iteration point $\mathbf{x}^{(k+1)}$.

Inner iterations to obtain conservatism

Let (k, ℓ) denote the ℓ:th inner iteration within the k:th outer iteration. The corresponding approximating functions are

$$\tilde{f}_i^{(k,\ell)}(\mathbf{x}) = f_i(\mathbf{x}^{(k)}) + \nabla f_i(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_i^{(k,\ell)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2,$$

and the corresponding approximating subproblem is

$$\begin{aligned} &\text{minimize} \quad \tilde{f}_0^{(k,\ell)}(\mathbf{x}) \\ &\text{subject to} \quad \tilde{f}_i^{(k,\ell)}(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m, \end{aligned}$$

with a unique optimal solution denoted $\hat{\mathbf{x}}^{(k,\ell)}$.

If $\tilde{f}_i^{(k,\ell)}(\hat{\mathbf{x}}^{(k,\ell)}) \geq f_i(\hat{\mathbf{x}}^{(k,\ell)})$ for all i, let $\mathbf{x}^{(k+1)} = \hat{\mathbf{x}}^{(k,\ell)}$.

Repeated inner iterations

Otherwise, let

$$\rho_i^{(k,\ell+1)} = \begin{cases} 1.1\,\tilde{\rho}_i^{(k,\ell)} & \text{if} \quad \tilde{f}_i^{(k,\ell)}(\hat{\mathbf{x}}^{(k,\ell)}) < f_i(\hat{\mathbf{x}}^{(k,\ell)}), \\ \rho_i^{(k,\ell)} & \text{if} \quad \tilde{f}_i^{(k,\ell)}(\hat{\mathbf{x}}^{(k,\ell)}) \geq f_i(\hat{\mathbf{x}}^{(k,\ell)}), \end{cases}$$

where $\tilde{\rho}_i^{(k,\ell)}$ is chosen such that

$$f_i(\mathbf{x}^{(k)}) + \nabla f_i(\mathbf{x}^{(k)})(\hat{\mathbf{x}}^{(k,\ell)} - \mathbf{x}^{(k)}) + \tilde{\rho}_i^{(k,\ell)} \|\hat{\mathbf{x}}^{(k,\ell)} - \mathbf{x}^{(k)}\|^2 = f_i(\hat{\mathbf{x}}^{(k,\ell)}),$$

i.e., $\tilde{\rho}_i^{(k,\ell)} = \rho_i^{(k,\ell)} + \dfrac{f_i(\hat{\mathbf{x}}^{(k,\ell)}) - \tilde{f}_i^{(k,\ell)}(\hat{\mathbf{x}}^{(k,\ell)})}{\|\hat{\mathbf{x}}^{(k,\ell)} - \mathbf{x}^{(k)}\|^2} > \rho_i^{(k,\ell)}$.

Then solve the new subproblem to obtain $\hat{\mathbf{x}}^{(k,\ell+1)}$, etc.

Summary of the k:th outer iteration

Starting from the (feasible) iteration point $\mathbf{x}^{(k)}$, the next (feasible) iteration point $\mathbf{x}^{(k+1)}$ is obtained as the optimal solution to the final of one or several subproblems of the type

$$\begin{aligned}
\text{minimize} \quad & f_0(\mathbf{x}^{(k)}) + \nabla f_0(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_0^{(k,\ell)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2 \\
\text{subject to} \quad & f_i(\mathbf{x}^{(k)}) + \nabla f_i(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_i^{(k,\ell)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2 \leq 0, \\
& i = 1, \ldots, m,
\end{aligned}$$

where the only difference between two consecutive subproblems is that some parameters $\rho_i^{(k,\ell)}$ have increased.

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Sufficient assumptions to ensure convergence

Let $\mathcal{F} = \{\, \mathbf{x} \in R^n \mid f_i(\mathbf{x}) \leq 0, i = 1, \ldots, m \,\}$.

For $\mathbf{x} \in \mathcal{F}$, let $\mathcal{A}(\mathbf{x}) = \{\, i \in \{1, \ldots, m\} \mid f_i(\mathbf{x}) = 0 \,\}$.

Assumptions:

- The feasible set $\mathcal{F}$ is nonempty and bounded.
- A feasible point $\mathbf{x}^{(1)} \in \mathcal{F}$ is known (or can be calculated).
- $f_0, f_1, \ldots f_m$ have continuous second derivatives on $\mathcal{F}$.
- Each feasible point $\mathbf{x} \in \mathcal{F}$ is a regular point, i.e. the gradients of the active constraints at $\mathbf{x}$ are positive-linearly independent, i.e. there are no numbers λ_i such that

$$\sum_{i \in \mathcal{A}(\mathbf{x})} \lambda_i \nabla f_i(\mathbf{x}) = \mathbf{0}^{\mathsf{T}}, \quad \sum_{i \in \mathcal{A}(\mathbf{x})} \lambda_i > 0, \quad \text{and} \quad \lambda_i \geq 0, \; i \in \mathcal{A}(\mathbf{x}).$$

Preparatory results

Propositions:

- The considered problem (to minimize $f_0(\mathbf{x})$ s.t. $\mathbf{x} \in \mathcal{F}$) has at least one optimal solution, and each optimal solution is a KKT point. In particular, the set of KKT points is non-empty.
- Within each outer iteration, a finite number of inner iterations is needed until the subproblem becomes conservative.
- Each iteration point $\mathbf{x}^{(k)}$ is a feasible solution, i.e. $\mathbf{x}^{(k)} \in \mathcal{F}$.
- Unless $\mathbf{x}^{(k)}$ is already a KKT point of the original problem, the objective value at $\mathbf{x}^{(k+1)}$ is strictly better than the objective value at $\mathbf{x}^{(k)}$, i.e. $f_0(\mathbf{x}^{(k+1)}) < f_0(\mathbf{x}^{(k)})$.

Global convergence theorem

Let Ω denote the set of KKT points to the original problem. (Note that Ω is non-empty according to above.)

Further, let $\| \, \Omega - \mathbf{x}^{(k)} \, \|$ denote the *distance* from the set Ω to the iteration point $\mathbf{x}^{(k)}$, i.e. $\| \, \Omega - \mathbf{x}^{(k)} \, \| \; = \inf_{\mathbf{x} \in \Omega} \{ \, \| \, \mathbf{x} - \mathbf{x}^{(k)} \| \, \}$.

Theorem: $\| \, \Omega - \mathbf{x}^{(k)} \, \| \longrightarrow 0$ as $k \longrightarrow \infty$.

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Extended/restricted problem formulation

From now on, the following problem formulation is considered

$$
\begin{aligned}
\text{minimize} \quad & f_0(\mathbf{x}) + \sum_{i=1}^{m} (c_i y_i + \tfrac{1}{2} d_i y_i^2) \\
\text{subject to} \quad & f_i(\mathbf{x}) - y_i \leq 0, \quad i = 1, \ldots, m \\
& \mathbf{x} \in X, \;\; \mathbf{y} \geq \mathbf{0},
\end{aligned}
$$

where

- $X = \{\, \mathbf{x} \in R^n \mid x_j^{\min} \leq x_j \leq x_j^{\max},\; j = 1, \ldots, n \,\}$,
- $c_i \geq 0,\;\; d_i > 0,\;\; x_j^{\min} < x_j^{\max}$,
- $f_0, \ldots, f_m$ have continuous second derivatives on X.

Some properties of the considered problem

Some theoretical properties of the considered problem

$$\begin{aligned} \text{minimize} \quad & f_0(\mathbf{x}) + \sum_{i=1}^{m} (c_i y_i + \tfrac{1}{2} d_i y_i^2) \\ \text{subject to} \quad & f_i(\mathbf{x}) - y_i \le 0, \quad i = 1, \dots, m \\ & \mathbf{x} \in X, \quad \mathbf{y} \ge \mathbf{0}. \end{aligned}$$

- There are always feasible solutions to this problem.
- There is always at least one globally optimal solution.
- Each feasible solution is a regular point.
- Each optimal solution (local or global) is a KKT point.

Inner and outer iterations

As before, (k,ℓ) denotes the ℓ:th inner iteration within the k:th outer iteration. The corresponding approximating subproblem is

$$\begin{aligned} \text{minimize} \quad & \tilde{f}_0^{(k,\ell)}(\mathbf{x}) + \sum_{i=1}^{m} (c_i y_i + \tfrac{1}{2} d_i y_i^2) \\ \text{subject to} \quad & \tilde{f}_i^{(k,\ell)}(\mathbf{x}) - y_i \leq 0, \quad i = 1, \ldots, m \\ & \mathbf{x} \in X, \;\; \mathbf{y} \geq \mathbf{0}, \end{aligned}$$

where, as before, the approximating functions could be

$\tilde{f}_i^{(k,\ell)}(\mathbf{x}) = f_i(\mathbf{x}^{(k)}) + \nabla f_i(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) + \rho_i^{(k,\ell)} \|\mathbf{x} - \mathbf{x}^{(k)}\|^2$.

But other choices might be better for some classes of problems!

Approximating functions in MMA

In the method of moving asymptotes, MMA, the convex approximating functions are chosen as

$$\tilde{f}_i^{(k,\ell)}(\mathbf{x}) = \sum_{j=1}^{n} \left(\frac{p_{ij}^{(k,\ell)}}{u_j^{(k)} - x_j} + \frac{q_{ij}^{(k,\ell)}}{x_j - v_j^{(k)}} \right) + r_i^{(k,\ell)},$$

where $u_j^{(k)}$ and $v_j^{(k)}$ are parameters satisfying $v_j^{(k)} < x_j^{(k)} < u_j^{(k)}$, defining vertical asymptotes.

The coefficients $p_{ij}^{(k,\ell)} > 0$, $q_{ij}^{(k,\ell)} > 0$ and $r_i^{(k,\ell)}$ are chosen such that $\tilde{f}_i^{(k,\ell)}(\mathbf{x}^{(k)}) = f_i(\mathbf{x}^{(k)})$ and $\nabla \tilde{f}_i^{(k,\ell)}(\mathbf{x}^{(k)}) = \nabla f_i(\mathbf{x}^{(k)})$.

Approximating subproblem in MMA

The MMA subproblem thus looks as follows:

$$\text{minimize} \quad \sum_{j=1}^{n}\left(\frac{p_{0j}^{(k,\ell)}}{u_j^{(k)}-x_j}+\frac{q_{0j}^{(k,\ell)}}{x_j-v_j^{(k)}}\right)+r_0^{(k,\ell)}+\sum_{i=1}^{m}(c_i y_i+\tfrac{1}{2}d_i y_i^2)$$

$$\text{subject to} \quad \sum_{j=1}^{n}\left(\frac{p_{ij}^{(k,\ell)}}{u_j^{(k)}-x_j}+\frac{q_{ij}^{(k,\ell)}}{x_j-v_j^{(k)}}\right)+r_i^{(k,\ell)}-y_i\leq 0,\;\; i=1,..,m$$

$$x_j^{\min}\leq x_j\leq x_j^{\max} \;\text{ and }\; v_j^{(k)}<x_j<u_j^{(k)},\;\; j=1,\ldots,n.$$

Easy to solve, e.g. by a dual method, due to the convexity and separability.

Default rules for updating the asymptotes

The first two outer iterations, when $k = 1$ and $k = 2$,

$$\begin{aligned} u_j^{(k)} + v_j^{(k)} &= 2x_j^{(k)}, \\ u_j^{(k)} - v_j^{(k)} &= x_j^{\max} - x_j^{\min}. \end{aligned}$$

In later outer iterations, when $k \geq 3$,

$$\begin{aligned} u_j^{(k)} + v_j^{(k)} &= 2x_j^{(k)}, \\ u_j^{(k)} - v_j^{(k)} &= \gamma_j^{(k)}(u_j^{(k-1)} - v_j^{(k-1)}), \end{aligned}$$

where

$$\gamma_j^{(k)} = \begin{cases} 0.7 & \text{if} \quad (x_j^{(k)} - x_j^{(k-1)})(x_j^{(k-1)} - x_j^{(k-2)}) < 0, \\ 1.2 & \text{if} \quad (x_j^{(k)} - x_j^{(k-1)})(x_j^{(k-1)} - x_j^{(k-2)}) > 0, \\ 1 & \text{if} \quad (x_j^{(k)} - x_j^{(k-1)})(x_j^{(k-1)} - x_j^{(k-2)}) = 0, \end{cases}$$

The coefficients $p_{ij}^{(k,\ell)}$, $q_{ij}^{(k,\ell)}$ and $r_i^{(k,\ell)}$

$$\tilde{f}_i^{(k,\ell)}(\mathbf{x}) = \sum_{j=1}^{n} \left(\frac{p_{ij}^{(k,\ell)}}{u_j^{(k)} - x_j} + \frac{q_{ij}^{(k,\ell)}}{x_j - v_j^{(k)}} \right) + r_i^{(k,\ell)}, \quad \text{where}$$

$$p_{ij}^{(k,\ell)} = (u_j^{(k)} - x_j^{(k)})^2 \left(\left(\frac{\partial f_i}{\partial x_j}(\mathbf{x}^{(k)}) \right)^+ + \frac{\rho_i^{(k,\ell)}}{u_j^{(k)} - v_j^{(k)}} \right),$$

$$q_{ij}^{(k,\ell)} = (x_j^{(k)} - v_j^{(k)})^2 \left(\left(\frac{\partial f_i}{\partial x_j}(\mathbf{x}^{(k)}) \right)^- + \frac{\rho_i^{(k,\ell)}}{u_j^{(k)} - v_j^{(k)}} \right),$$

and $r_i^{(k,\ell)}$ is chosen such that $\tilde{f}_i^{(k,\ell)}(\mathbf{x}^{(k)}) = f_i(\mathbf{x}^{(k)})$.

Here, $\rho_0^{(k,\ell)} > 0$ and $\rho_i^{(k,\ell)} \geq 0$ for $i = 1, \ldots, m$.

Summary of the k:th outer iteration in MMA

Given the iteration point $(\mathbf{x}^{(k)}, \mathbf{y}^{(k)})$, the next iteration point $(\mathbf{x}^{(k+1)}, \mathbf{y}^{(k+1)})$ is obtained as the optimal solution to the final of one or several subproblems of the type

$$\text{minimize} \quad \sum_{j=1}^{n} \left(\frac{p_{0j}^{(k,\ell)}}{u_j^{(k)} - x_j} + \frac{q_{0j}^{(k,\ell)}}{x_j - v_j^{(k)}} \right) + r_0^{(k,\ell)} + \sum_{i=1}^{m} (c_i y_i + \tfrac{1}{2} d_i y_i^2)$$

$$\text{subject to} \quad \sum_{j=1}^{n} \left(\frac{p_{ij}^{(k,\ell)}}{u_j^{(k)} - x_j} + \frac{q_{ij}^{(k,\ell)}}{x_j - v_j^{(k)}} \right) + r_i^{(k,\ell)} - y_i \leq 0, \;\; i = 1,..,m$$

$$x_j^{\min} \leq x_j \leq x_j^{\max} \;\text{ and }\; v_j^{(k)} < x_j < u_j^{(k)}, \;\; j = 1, \ldots, n.$$

Before each outer iteration, $f_i(\mathbf{x}^{(k)})$ and $\nabla f_i(\mathbf{x}^{(k)})$ are needed.
After each inner iteration, $f_i(\hat{\mathbf{x}}^{(k,\ell)})$ is needed, but no gradients.

Global convergence

Let Ω denote the set of KKT points $(\mathbf{x}, \mathbf{y})$ to the considered problem

$$\begin{aligned} \text{minimize} \quad & f_0(\mathbf{x}) + \sum_{i=1}^{m} (c_i y_i + \tfrac{1}{2} d_i y_i^2) \\ \text{subject to} \quad & f_i(\mathbf{x}) - y_i \le 0, \quad i = 1, \ldots, m \\ & \mathbf{x} \in X, \;\; \mathbf{y} \ge \mathbf{0}. \end{aligned}$$

Theorem: $\| \, \Omega - (\mathbf{x}^{(k)}, \mathbf{y}^{(k)}) \, \| \longrightarrow 0$ as $k \longrightarrow \infty$.

Implementations in Matlab and Fortran

In our *Matlab* implementation, the convex subproblems are solved by a *primal-dual interior-point method*.

In our *Fortran* implementation, the convex subproblems are solved by an active-set Newton method applied to the *dual* problem.

M-files in Matlab and a source code in Fortran are available for academic research and education. Just send an e-mail.

Thank You!