Optimization and feasibility problems with expensive functions

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Outline

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What are Expensive Functions?

Expensive functions are in general time-consuming or cost-intensive black-boxes, e.g.

- simulations,
- experiments or
- applications of algorithms to a testset.

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- applications of algorithms to a testset.

$\Rightarrow$ No derivative information available.
$\Rightarrow$ Avoid evaluations of expensive functions whenever possible.

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Expensive Feasibility and Optimization Problem

nonlinear feasibility
problem (EFP)

$$c_{\mathcal{I}}(x, u(x)) \leq 0$$
$$c_{\mathcal{E}}(x, u(x)) = 0$$
$$x \in \mathbb{R}^n$$

u : expensive function (sufficiently smooth)

$c_{\mathcal{I}}, c_{\mathcal{E}}$: twice continuously differentiable

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nonlinear constrained optimization problem (EOP)

$$\begin{aligned} \min\ & f(x, u(x)) \\ \text{s.t. } & c_{\mathcal{I}}(x, u(x)) \leq 0 \\ & c_{\mathcal{E}}(x, u(x)) = 0 \\ & x \in \mathbb{R}^n \end{aligned}$$

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Reformulation: Sequence of Cheap Systems

nonlinear feasibility problem (EFP)

$$c_{\mathcal{I}}(x, m_k^u(x)) \leq 0$$
$$c_{\mathcal{E}}(x, m_k^u(x)) = 0$$
$$x \in \mathcal{Q}_k(x_k, \delta_k)$$

m_k^u : model of the expensive function in iteration k

$\mathcal{Q}_k$: trust region $\mathcal{Q}_k(x_k, \delta_k) := \{x \in \mathbb{R}^n \mid \|x - x_k\| \leq \delta_k\}$

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Properties of the Model m_k^u

- linear function
  ($n + 1$ sample points $\overline{X} = \{\bar{x}_0, \ldots, \bar{x}_n\} \subset \mathcal{Q}_k$, $x_k \in \overline{X}$)

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- based on Lagrange basis polynomials

$$m_k^u(x) = \sum_{i=0}^{n} u(\bar{x}_i) L_i(x)$$

with

$$L_i(x) = \begin{cases} 1 & \text{if} \quad x = \bar{x}_i \\ 0 & \text{if} \quad x \in \overline{X} \setminus \{\bar{x}_i\} \end{cases}$$

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- Λ-poisedness of the sample points, i.e.

$$\max_{i=0,\ldots,n} \max_{x \in \mathcal{Q}(x_k, \delta_k)} |L_i(x)| \leq \Lambda$$

  can be verified and established if neccessary

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Least-Squares Reformulation of (EFP)

Find a (local) minimum of the unconstrained problem

$$\min_{x \in \mathbb{R}^n} \quad f(x, u(x)) \quad = \quad \tfrac{1}{2}\|\vartheta(x, u(x))\|_2^2$$

where

$$\vartheta(x, u(x)) := \begin{pmatrix} c_{\mathcal{E}}(x, u(x)) \\ [c_{\mathcal{I}}(x, u(x))]_+ \end{pmatrix} \in \mathbb{R}^{p+q}$$

is the vector of violations of the equations and inequalities.

Trust-Region Subproblem of (EFP)

Find a (local) minimum of the constrained problem

$$\min_{x \in \mathbb{R}^n} \; f(x, m_k^u(x))$$
$$\text{s.t. } \; x \in \mathcal{Q}(x_k, \delta_k)$$

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$$f(x, m_k^u(x)) = \frac{1}{2} \|\vartheta(x, m_k^u(x))\|_2^2$$
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Basic Ideas

- expensive function
  - ⇒ Λ-poised interpolation models by Conn, Scheinberg, Vicente (2009)
  - ⇒ conditional trust-region algorithm by Conn, Gould, Toint (2000)
- general nonlinear system of equations and inequalities
  - ⇒ filter trust-region algorithm FILTRANE by Gould, Toint (2007)
- general nonlinear constrained optimization problem
  - ⇒ trust-region SQP-filter algorithm by Fletcher, Gould, Leyffer, Toint, Wächter (2002)
- general nonlinear trust-region subproblem
  - ⇒ subproblem solver needs to satisfy the sufficient model decrease condition

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Outline of EFNES

Step 0: Initialization

Step 1: Stopping test

Step 2: Trial point determination

Step 3: Acceptance of the trial point

Step 4: Model improvement

Step 5: Selection of new iterate

Step 6: Acceptance test

Step 7: Trust region update

Outline of EFNES

Step 0: Initialization

Input initial values for parameters and compute m_k^0 and $c_0 = c(x_0, u(x_0))$.

Step 1: Stopping test

Step 2: Trial point determination

Step 3: Acceptance of the trial point

Step 4: Model improvement

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Outline of EFNES

Step 0: Initialization

Step 1: Stopping test

Stop if $\vartheta(x_k, u(x_k)) = 0$ or $\|\nabla f(x_k)\|_2 < \varepsilon$ for a valid m_k^u.
If m_k^u is not valid improve the model.

Step 2: Trial point determination

Step 3: Acceptance of the trial point

Step 4: Model improvement

Step 5: Selection of new iterate

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Outline of EFNES

Step 0: Initialization

Step 1: Stopping test

Step 2: Trial point determination

Try to compute x_k^+ which provides a sufficent model decrease.
If this is not possible improve the model and go to Step 1.

Step 3: Acceptance of the trial point

Step 4: Model improvement

Step 5: Selection of new iterate

Step 6: Acceptance test

Step 7: Trust region update

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Outline of EFNES

Step 0: Initialization

Step 1: Stopping test

Step 2: Trial point determination

Step 3: Acceptance of the trial point

If the ratio of predicted (by m_k^u) and actual (requires evaluation of $u(x_k^+)$) improvement is "good enough" accept the trial point.

Step 4: Model improvement

Step 5: Selection of new iterate

Step 6: Acceptance test

Step 7: Trust region update

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Outline of EFNES

Step 0: Initialization

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Step 4: Model improvement

If neccessary improve m_k^u (dependent on the quality of its prediction). Consider arising alternatives for the trial point.

Step 5: Selection of new iterate

Step 6: Acceptance test

Step 7: Trust region update

Outline of EFNES

Step 0: Initialization

Step 1: Stopping test

Step 2: Trial point determination

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Step 5: Selection of new iterate

Choose the best candidate among x_k^+ and the points generated during the improvement of the model as final trial point x_k^*.

Step 6: Acceptance test

Step 7: Trust region update

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Outline of EFNES

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Decide if x_k^* is accepted as x_{k+1} dependent on the accuracy of the prediction by the model in x_k^* and some additional criterion.

Step 7: Trust region update

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Step 7: Trust region update

Update the radius of the trust-region according to the accuracy of the model if the trust-region was used in the current iteration.

Assumptions 1 - 6

1. $c_{\mathcal{I}}$, $c_{\mathcal{E}}$, u twice continuously differentiable, bounded from above
2. iterates remain in bounded domain
3. m_k^u twice continuously differentiable
4. error bounds on model m_k^u
5. check and guarantee model validity, whenever necessary
6. the solver for the TR-subproblem achieves a sufficient model decrease

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Global Convergence of EFNES

Theorem

Suppose that Assumptions 1-6 hold. Then either

$$\|\nabla f(x_k, u(x_k))\|_2 = 0$$

for some finite k or

$$\lim_{k \to \infty} \|\nabla f(x_k, u(x_k))\|_2 = 0.$$

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Moreover, if infinitely many values are added to the filter, then we have that

$$\lim_{k\to\infty} \|\vartheta(x_k, u(x_k))\|_2 = 0.$$

Test Environment

Testset:

- 54 small and medium sized test problems from the CUTEr library
- randomly selected parts are treated as expensive functions

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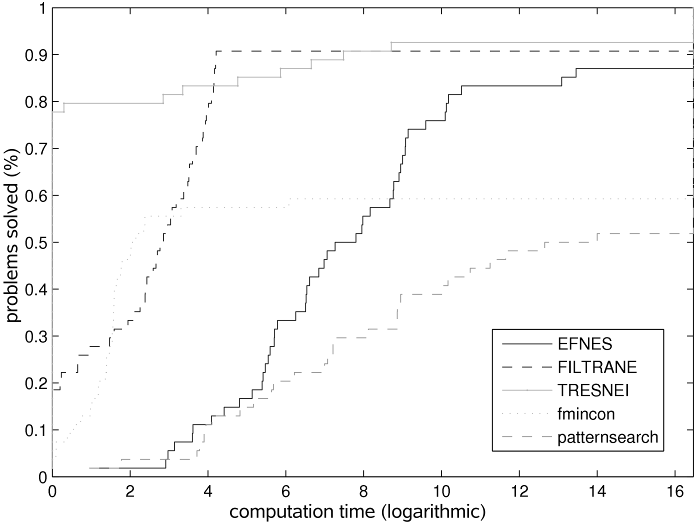
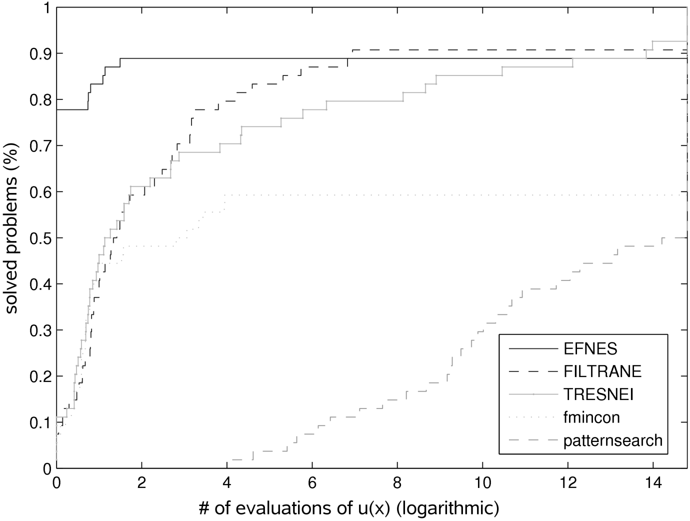
Compared methods:

- Matlab implementation of EFNES
- Matlabfunctions *fmincon* and *patternsearch* (from the optimization- and direct-search toolbox, respectively)
- TRESNEI (Filter-Trust-Region based solver for nonlinear systems of (in-)equalities by Morini and Porcelli, 2009)
- FILTRANE (part of the Galahad toolbox by Gould, Orban and Toint, 2007)

Performance Profile Comparing Computation Time



Performance Profile Comparing the Number of Evaluations of the Expensive Function



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Thank you for your attention!

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