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The MADS algorithm: dealing with general equality constraints; Discussions

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Introduction

The problem

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

with

- $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ the objective function.
- $c_j : \mathbb{R}^n \to \mathbb{R}$, $j \in \mathcal{I}$ the set of $|\mathcal{I}|$ inequality constraints ($|\mathcal{I}| \geq 0$)
- $c_j : \mathbb{R}^n \to \mathbb{R}$, $j \in \mathcal{E}$ the set of $|\mathcal{E}|$ equality constraints ($|\mathcal{E}| \geq 0$).
- $l, u \in \mathbb{R}^n$ the bound constraints on the variables (can be equal to $\pm\infty$ as long as $l_i < u_i$ for $i = 1, 2, \ldots, n$).

The functions f and c_j for $j \in \mathcal{E} \cup \mathcal{I}$ are supposed to be blackboxes (ideally).

The MADS algorithm

MADS (Mesh Adaptive Direct Search) [Audet and Dennis, 2006] is an iterative (and robust) method which:

- Evaluates points on a mesh.
- Iterates around two steps: the search (optional) and the poll.
- Is guaranteed to converge to a local optimum under rather general assumptions (i.e. locally Lipschitz functions).

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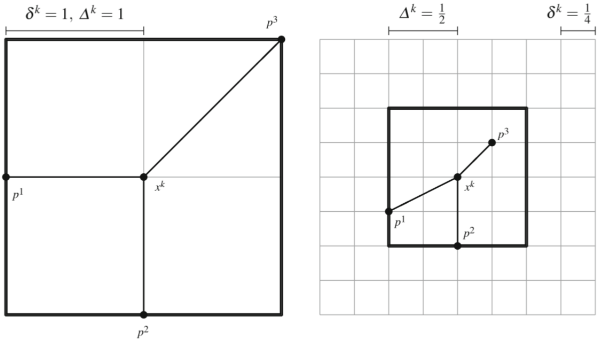

The MADS algorithm and inequality constraints

The constraint violation function h [Audet and Dennis, 2009]

The constraint violation function $h : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is defined as

$$h(x) = \begin{cases} \sum_{j \in \mathcal{I}} \max(g_j(x), 0)^2 & \text{if } x \in X; \\ 0 & \text{otherwise} \end{cases}$$

where X is the set of relaxable constraints.

The PB-MADS algorithm [Audet and Dennis, 2009] deals with inequality constraints:

- Via the use of the constraint violation h. At iteration k, all points above the threshold $h^k_{\max}$ are rejected
- Each iteration is organized around a poll and a search (optional).
- At each iteration, keeps a list of non-infeasible incumbents points and iterates around them.
- $h^k_{\max}$ decreases toward the iterations.

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A question

Are you a bit familiar with the notion of manifold ?

A question

Are you familiar with the notion of linear programming ?

Blackbox optimization on manifolds

Definition

In mathematics, a manifold is a topological space that locally resembles Euclidean space near each point. More precisely, an n-dimensional manifold, or n-manifold for short, is a topological space with the property that each point has a neighborhood that is homeomorphic to the Euclidean space of dimension n. ***Wikipedia***

Requires

- The (analytical) knowledge of equality constraints.
- A transformation mapping to solve the problem in a reduced dimension subspace.

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Example

Solve the following equality constraint blackbox problem

$$\begin{array}{ll} \min\limits_{(x_1,x_2)\in\mathbb{R}^2} & f(x_1,x_2) \\ \text{s.t} & x_1^2 + x_2^2 = 1 \end{array}$$

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Blackbox optimization on manifolds

General litterature

- Direct search methods on Riemannian manifolds [Dreisigmeyer, 2006a, Dreisigmeyer, 2006b, Dreisigmeyer, 2007b].
- Direct search methods over Lipschitz manifolds [Dreisigmeyer, 2007a].
- Other [Dreisigmeyer, 2018, Dreisigmeyer, 2019].

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- Other [Dreisigmeyer, 2018, Dreisigmeyer, 2019].

More specific

- Direct search methods with linear equality constraints [Audet et al., 2015, Lewis et al., 2006, Lewis and Torczon, 2010].
- Direct search methods with spherical inequality constraints [Latorre et al., 2018].

A simple method

Reformulate the equality constrained problem as an inequality constrained problem

$$\begin{array}{ll} \min\limits_{x\in\mathbb{R}^n} & f(x) \\ \text{s.t} & c_{\mathcal{I}}(x) \leq 0 \\ & c_{\mathcal{E}}(x) = 0 \\ & l \leq x \leq u \end{array} \implies \begin{array}{ll} \min\limits_{x\in\mathbb{R}^n} & f(x) \\ \text{s.t} & c_{\mathcal{I}}(x) \leq 0 \\ & c_{\mathcal{E}}(x) \leq 0 \text{ and } c_{\mathcal{E}}(x) \geq 0 \\ & l \leq x \leq u \end{array}$$

A simple method

Reformulate the equality constrained problem as an inequality constrained problem

$$
\begin{array}{ll}
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\end{array}
$$

Inspiration

Engineering common sense.

A simple method

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Inspiration

Engineering common sense.

Problem

- Scaling: the algorithm can reject many points when the domain is too narrow.
- Theory.

Extension of the constraint violation function to equality constraints

Inspiration

[Nocedal and Wright, 2006, Chapter 15]

Extend the constraint violation function for equality constrained problems

The constraint violation function $h : \mathbb{R}^n \to \mathbb{R} \cup +\infty$ is defined as

$$h(x) = \begin{cases} \sum_{j \in \mathcal{I}} \max(c_j(x), 0)^2 + \sum_{j \in \mathcal{E}} c_j(x)^2 & \text{if } x \in X \\ 0 & \text{otherwise} \end{cases}$$

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Problem

- Equivalent to the first approach.

ε approach/restoration methods for derivative free optimization

Litterature

- General framework [Martínez and Sobral, 2013].
- Use of GSS [Bueno et al., 2013]
- Use of derivative-free trust regions [Arouxét et al., 2015, Echebest et al., 2017]

General principle [Martínez and Sobral, 2013]

An iteration k is decomposed into two phases:

- The Restoration phase. Find a point $y^k \in \Omega$ satisfying the following condition

$$\|c_{\mathcal{E}}(y^k)\| \leq \varepsilon^k$$

  where $\Omega = \{x \in \mathbb{R}^n : l \leq x \leq u \text{ and } c_{\mathcal{I}}(x) \leq 0\}$
- The Optimization phase. Starting from y^k, solve approximatively the following problem

$$\begin{array}{ll} \min\limits_{x \in \Omega} & f(x) \\ \text{s.t} & \|c_{\mathcal{E}}(x)\| \leq \varepsilon^k \end{array}$$

- Update ε^k to $\varepsilon^{k+1} > 0$, set $k \to k+1$ and repeat the two steps above.

ε approach/restoration methods for derivative free optimization

Some remarks

- One can have one ε_i^k by equality constraints, i.e. $\varepsilon^k \in \mathbb{R}_+^p$.
- The two phases can be tackled by different algorithms, according to the nature of the constraints (i.e. for example c_j differentiable and/or cheap constraints [Bueno et al., 2013, Martínez and Sobral, 2013])
- Some variants solve a penalty subproblem in the Optimization phase mixing constraints and objective functions [Arouxét et al., 2015, Echebest et al., 2017].

The penalty function [Bueno et al., 2013]

Given $\theta \in (0,1)$, define the following penalty function:

$$\phi(x,\theta) = \theta\ f(x) + (1-\theta)\|c_{\mathcal{E}}(x)\|$$

ε approach/restoration methods for derivative free optimization

A very dumb idea (inspired by [Bueno et al., 2013, Martínez and Sobral, 2013])

- **Initialization**. Let $x^0 \in [l, u]$ a starting point. Set $k := 0$ and $\theta^0 \in (0, 1)$.
- **Step 1 : Restoration phase**. If $\|c_{\mathcal{E}}(x^k)\| = 0$, set $y^k := x^k$, and go to Step 2. Else, execute a Mads iteration around x^k to find a point y^k satisfying $\|c_{\mathcal{E}}(y^k)\| < \|c_{\mathcal{E}}(x^k)\|$. If success, go to Step 2. Otherwise, go to Step 4.
- **Step 2: Update penalty parameter**. If $\phi(y^k, \theta^k) - \phi(x^k, \theta^k) \leq \frac{1}{2}(\|c_{\mathcal{E}}(y^k)\| - \|c_{\mathcal{E}}(x^k)\|)$, set $\theta^{k+1} := \theta^k$. Otherwise, set

$$\theta^{k+1} := \frac{\|c_{\mathcal{E}}(x^k)\| - \|c_{\mathcal{E}}(y^k)\|}{2(f(y^k) - f(x^k) + \|c_{\mathcal{E}}(x^k)\| - \|c_{\mathcal{E}}(y^k)\|)}$$

- **Step 3 : Optimization phase**. Execute a Mads iteration around y^k to find point x^{trial} such that

$$\phi(x^{trial}, \theta^{k+1}) - \phi(x^k, \theta^{k+1}) \leq \frac{1}{2}(\|c_{\mathcal{E}}(x^k)\| - \|(c_{\mathcal{E}}(y^k)\|).$$

  If x^{trial} satisfies the conditions, set $x^{k+1} := x^{trial}$; otherwise set $x^{k+1} := y^k$. Go to Step 4.
- **Step 4: Update parameter**. Update the mesh size and frame size parameter as for the traditional MADS algorithm. Set $k := k + 1$.

Penalty function approach

Litterature

- Exact penalty methods (for inequality constraints): [Di Pillo et al., 2016, Fasano et al., 2014, Liuzzi and Lucidi, 2009].
- Non exact penalty methods: [Griffin and Kolda, 2010, Price, 2020]

Idea

$$\begin{array}{ll} \min\limits_{x \in \mathbb{R}^n} & f(x) \\ \text{s.c} & c_{\mathcal{I}}(x) \leq 0 \\ & c_{\mathcal{E}}(x) = 0 \\ & l \leq x \leq u \end{array} \Longrightarrow \min_{x \in [l,u]} Z_1(x,\rho) \text{ or } \min_{x \in [l,u]} Z_2(x,\rho)$$

where

$$Z_1(x,\rho) = f(x) + \rho \left(\sum_{j \in \mathcal{I}} \max(0, c_j(x)) + \sum_{j \in \mathcal{E}} |c_j(x)| \right), \rho > 0$$

and

$$Z_2(x,\rho) = f(x) + \rho \left(\sum_{j \in \mathcal{I}} \max(0, c_j(x))^2 + \sum_{j \in \mathcal{E}} c_j(x)^2 \right), \rho > 0.$$

Penalty function approach

Remarks

- One can also let the inequality constraints in the original constraints.
- In derivative-free optimization literature, convergence results have been given in the case where:
  1. The objective function and the inequality constraints (no equality constraints) are Lipschitz continuous [Di Pillo et al., 2016] for the l_1 penalty function.
  2. The exactness of the l_1 penalty function has been equally proved in the case where the objective function and the constraints functions are locally Lipschitz (ϕ, η) invex [Antczak, 2019].

Penalty function approach variant

Idea (given by Orban/Conn)

Reformulate the original problem:

$$\begin{array}{ll} \min\limits_{x \in \mathbb{R}^n, s \in \mathbb{R}^p_+} & f(x) + \rho \sum_{i=1}^{p} s_i \\ \text{s.t} & c_{\mathcal{I}}(x) \leq 0 \\ & -s_i \leq c_i(x) \leq s_i, i \in \mathcal{E} \\ & l \leq x \leq u. \end{array}$$

with $\rho > 0$ a fixed real parameter. Two ways to solve it:

- Solve the $n + p$ inequality constrained problem with progressive barrier.
- We only consider the x variables. The s slack variables are directly adjusted into the blackbox.

Augmented Lagrangian

Litterature

- Direct search methods [Gramacy et al., 2016, Lewis and Torczon, 2002, Lewis et al., 2006, Lewis and Torczon, 2010]
- Trust region methods [Audet et al., 2016, Diniz-Ehrhardt et al., 2011]
- Surrogate-based methods [Picheny et al., 2016]

Augmented Lagrangian

Augmented Lagrangian definition

- "Classical" formulation [Nocedal and Wright, 2006]

$$\mathcal{L}(x;\lambda,\rho) = f(x) + \sum_{j\in\mathcal{E}} \lambda_j c_j(x) + \frac{\rho}{2}\sum_{j\in\mathcal{E}} |c_j(x)|^2,$$

  used in [Lewis and Torczon, 2002, Lewis et al., 2006, Picheny et al., 2016].

- Powell-Hestenes-Rockafellar formulation [Andreani et al., 2008]

$$\mathcal{L}(x;\lambda,\mu,\rho) = f(x) + \frac{\rho}{2}\left(\|c_{\mathcal{E}}(x) + \lambda/\rho\|^2 + \|\max(0, c_{\mathcal{I}}(x) + \mu/\rho)\|^2\right)$$

  for $\lambda \in \mathbb{R}^{|\mathcal{E}|}, \mu \in \mathbb{R}_+^{|\mathcal{I}|}, \rho > 0$
  used in [Audet et al., 2016, Diniz-Ehrhardt et al., 2011, Lewis and Torczon, 2010].

Augmented Lagrangian

Basic framework [Lewis and Torczon, 2010]

- **Initialisation**: Let $x^0 \in \mathbb{R}^n \cap [l, u]$ be an initial point, $\rho^1 > 0$ and initialize $\mu^1 \in \mathbb{R}_+^{|\mathcal{I}|}$, $\lambda^1 \in \mathbb{R}^{|\mathcal{E}|}$, $\delta_{tol}^1 > 0$. Set $k := 1$ and $\sigma^0 := \max\left(0, c_{\mathcal{I}}(x^0)\right)$.
- **Step 1 : Solve the subproblem**

$$\begin{array}{ll} \min & \mathcal{L}(x; \lambda^k, \mu^k, \rho^k) \\ \text{s.t} & l \leq x \leq u \end{array}$$

  Stop when $\delta^{j_k} < \delta_{tol}^k$. Get x^k "solution" of this problem.
- **Step 2: Update the multipliers estimates**. Set $\lambda^{k+1} := \lambda^k + \rho^k c_{\mathcal{E}}(x^k)$; $\sigma^k := \max\left(c_{\mathcal{I}}(x^k), -\mu^k/\rho^k\right)$ and $\mu^{k+1} := \max\left(0, \mu^k + \rho^k c_{\mathcal{I}}(x^k)\right)$.
- **Step 4: Update the penalty parameters**. If

$$\max\left(\|c_{\mathcal{E}}(x^k)\|_\infty, \|\sigma^k\|_\infty\right) \leq (1/2)\max\left(\|c_{\mathcal{E}}(x^{k-1})\|_\infty, \|\sigma^{k-1}\|_\infty\right),$$

  set $\rho^{k+1} := \rho^k$; otherwise $\rho^{k+1} := 2\rho^k$.
- **Step 5: Fix new tolerance subproblem**. Choose $\xi \in (0, 1)$ and set

$$\delta_{tol}^{k+1} := \xi\delta^k / \max(1, (1 + \|\lambda^{k+1}\| + \|\mu^{k+1}\| + \rho^{k+1})/\epsilon_{tol}). \text{ Go to Step 1.}$$

Augmented Lagrangian

Remarks

- One is not forced to integrate the inequality constraints into the augmented Lagrangian.
- To think about: δ_{tol}^{k+1} is a decreasing parameter. Allow it to increase ?
- A subproblem execution = A Mads iteration ?
  [Audet et al., 2016, Picheny et al., 2016]

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