Blackbox Optimization using Mesh Adaptive Direct Search

MADS; method, algorithm and implementations

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Overview

- What is blackbox optimization?
- Functions differentiability
- Direct search methods
- Mesh adaptive direct search method
- Implementations
- Running example

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Blackbox Optimization Problems

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$$x \longrightarrow \boxed{\text{Blackbox}} \xrightarrow[x \in \Omega?]{f(x)}$$

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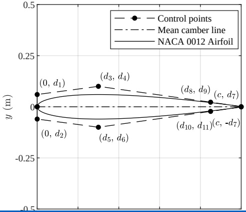
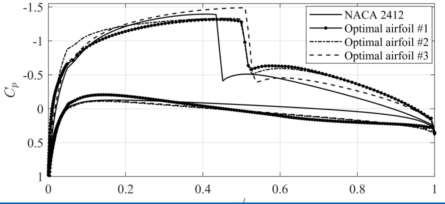
Transonic Airfoil shape optimization using TSFOIL, SU2, OpenFoam, fluent ...etc.





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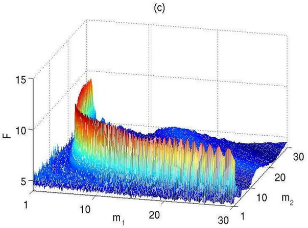
Each call to the simulation is time-consuming
Derivatives cannot be trusted or evaluated.



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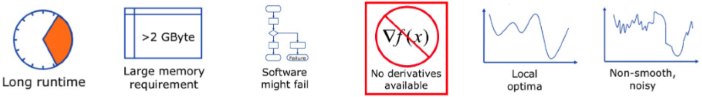
BBO challenges



Possible bad properties of a blackbox from *J. Simonis, 2009, The Boeing Company*

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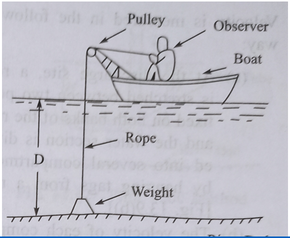
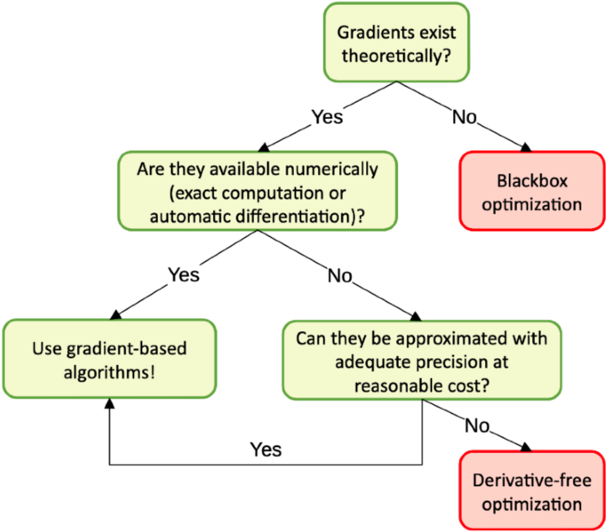
John Dennis analogy [Powell 1994]



Gradients availablity



Blackbox Optimization Problems

Definition: Blackbox optimization

It refers to problems where objective and constraint functions cannot be exploited.

Often the case when their evaluation requires the execution (usually time-consuming) simulation using computational models, typically inaccessible by the user.

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Definition: Derivative-free optimization

It refers to the use of algorithms that utilize only function values because their derivatives are either not defined or not available.

Gradient approximations may sometimes be obtained, but the amount of work required to ensure they are dependable may not be worth the effort.

Types of constraints

The domain: $\Omega = \{x \in X : c_j(x) \leq 0, j \in J\} \subset \mathbb{R}^n$

- The set X represents *unrelaxable constraints*
- $c_j(x) \leq 0$ are *relaxable constraints*
- *Hidden constraints*: when the simulation fails for points in Ω

Properties of a function

- We consider a function $f : \mathbb{R}^n \to \mathbb{R}$.
- We define some properties of f at x, a point of its domain.
- We say that these properties apply near x if the property is satisfied on some open neighborhood of x.
- We can also consider some properties on a domain $\mathcal{X} \subset \mathbb{R}^n$.
- f is continuous at $x \in \mathbb{R}^n$ if the limit $\lim_{y \to x} f(y)$ exists and is equal to $f(x)$.

Types of variables

The decision variables x can be any combination of

- Continuous $\mathbb{R}$
- Integer $\mathbb{N}$ or $\mathbb{Z}$
- binary $\{0,1\}$
- granular $\{0, 0.05, 0.10, ..., 0.95, 1.00\}$
- Categorical $\{0, 0.05, 0.10, ..., 0.95, 1.00\}$
  - Ex: Hyper-parameter optimization of deep neural network

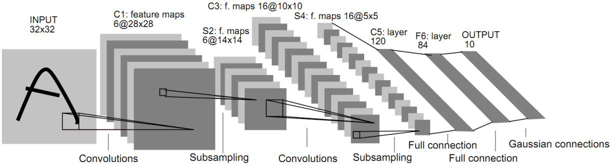

Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

- No ordinal property
- The number of convolution layers impacts the total number of optimization variables

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Differentiability

Consider the function $f : \mathbb{R}^n \to \mathbb{R}$.

- f is differentiable at $x \in \mathbb{R}^n$ if there exists $g \in \mathbb{R}^n$ such that

$$\lim_{y \to x} \frac{f(y) - f(x) - g^\top (y-x)}{\|y-x\|} = 0$$

- If this g exists, it is unique and is called the gradient of f at x, denoted $\nabla f(x)$.
- If f is differentiable at x, then f is continuous at x.
- Partial derivatives:

$$\nabla f(x) = \left(\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \dots, \frac{\partial f(x)}{\partial x_n} \right)^\top$$

Differentiability classes

- A function $f : \mathbb{R}^n \to \mathbb{R}$ is said of class $\mathcal{C}^k$, denoted $f \in \mathcal{C}^k$, with $0 \leq k \leq \infty$, if all the possible partial derivatives of the form

$$\frac{\partial^k f}{\partial x_{i_1} \partial x_{i_2} \cdots \partial x_{i_k}}$$

  exist and are continuous, where $i_\ell \in \{1, 2, \ldots, n\}$ for all $\ell \in \{1, 2, \ldots, k\}$.

- $\mathcal{C}^0$: Continuous functions.
- $\mathcal{C}^1$: Continuously differentiable functions.
- $\mathcal{C}^\infty$: Smooth functions.

Lipschitz functions

- f is Lipschitz on the set $\mathcal{X} \subset \mathbb{R}^n$ if there exists a scalar $K > 0$ such that

$$|f(x) - f(y)| \leq K\|x - y\| \text{ for all } x, y \in \mathcal{X}$$

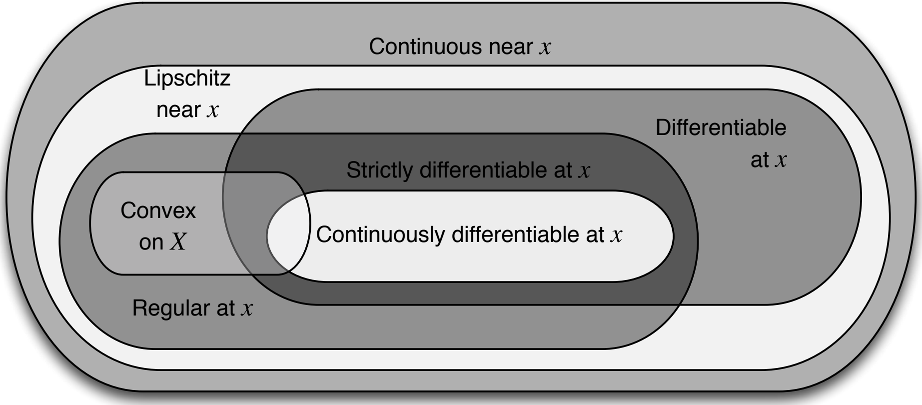
- K is called the Lipschitz constant.

- Examples of non-Lipschitz functions:
  - $f(x) = \sqrt{x}$ for $x \geq 0$.
  - Discontinuous functions, $\tan(x)$ for $x \in (-\pi/2, \pi/2)$, $\frac{1}{x}$ for $x \in \mathbb{R}$.
  - $f(x) = x^2$ for $x \in \mathbb{R}$.

  Examples of Lipschitz functions:
  - $f(x) = \sqrt{x^2 + 5}$ for $x \in \mathbb{R}$, $K = 1$.
  - $\sin(x)$ for $x \in \mathbb{R}$, $K = 1$.
  - $f(x) = |x|$ for $x \in \mathbb{R}$, $K = 1$.

Summary of function types

$f : X \subseteq \mathbb{R}^n \to \mathbb{R}$ is...



Convergence analysis (1/2)

- An optimization algorithm is not considered heuristic when it is backed by a convergence analysis which ensures some properties at the resulting solution $\hat{x}$.
- This analysis typically depends on some assumptions made about the nature of the problem. For example: differentiability of f, convexity of Ω, etc.
- Usually, these properties are given as necessary or sufficient optimality conditions.
- Recall that global convergence refers to independence of the starting point.

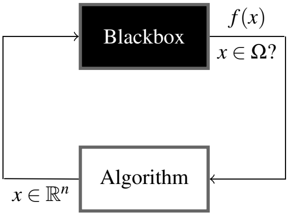
Convergence analysis (2/2)

- In DFO, we expect global convergence to solutions satisfying some local and necessary optimality conditions, when the function is supposed Lipschitz.
- However, a blackbox has no exploitable property and cannot be proven Lipschitz.
- **But** consider the following choice between two algorithms to apply to such a problem:
  - Algorithm $\mathcal{A}$ is a heuristic; it **may** yield a point $\hat{x}$ where $\nabla f(\hat{x}) \neq 0$ when f is differentiable.
  - Algorithm $\mathcal{B}$ guarantees $\nabla f(\hat{x}) = 0$ when f is differentiable.

  The choice is obvious.

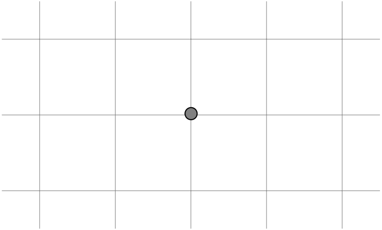
General scheme

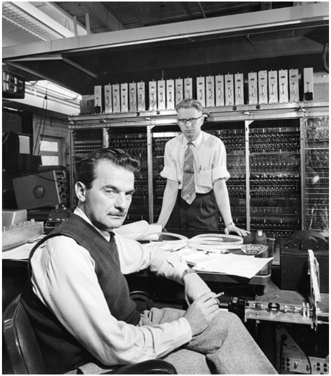
Direct search methods launch the blackbox simulation at tentative trial points in hopes of improving the current best solution.
* The way that the trial points are generated defines the method



Unconstrained optimization - Coordinate search

1952 Fermi and Metropolis
Coordinate Search algorithm.





Metropolis and Richardson in front of the MANIAC computer
Source http://www.ominous-valve.com/maniac.html

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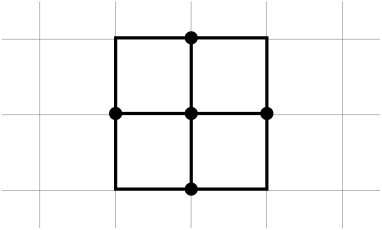

- INITIALIZATION:
  x_0 : starting point in $\mathbb{R}^n$
  $\Delta_0 > 0$: initial step size
- POLL STEP: for $k = 0, 1, \ldots$
  if $f(t) < f(x_k)$ for $t \in P_k := \{x_k \pm \Delta_k e_i : i = 1, 2, \ldots, n\}$:
  $x_{k+1} \leftarrow t$
  $\Delta_{k+1} \leftarrow \Delta_k$
  else (failure): x_k is a local minimum relatively to P_k:
  $x_{k+1} \leftarrow x_k$
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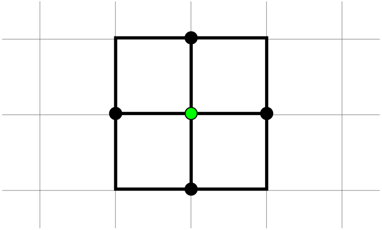

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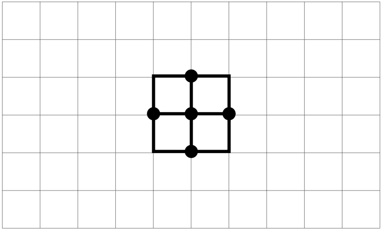

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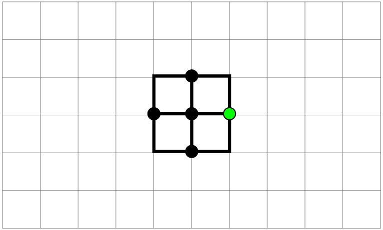

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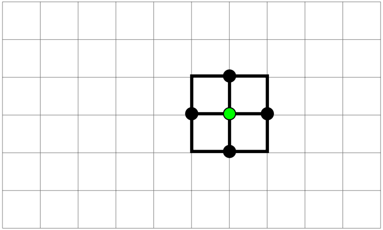

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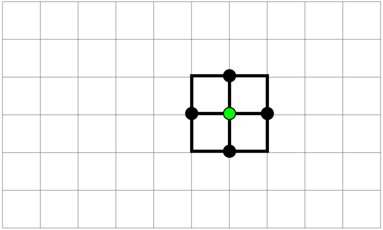

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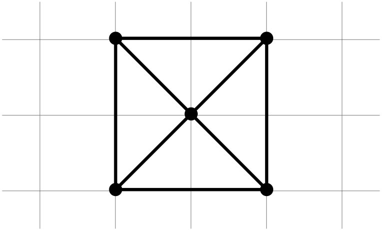
- Remarks
  - Evaluation of x_0 is counted
  - Extension with bounds: if the algorithm generates a trial point outside of the boundary, then do not evaluate and consider as failure
  - If the algorithm generates a trial point x found in the cache, then do not evaluate and consider as failure

CS variants

Complete			Opportunist			Ordered		
k	trial point $t^\top$	$f(t)$	k	trial point $t^\top$	$f(t)$	k	trial point $t^\top$	$f(t)$
0	$[3,2]$	29286	0	$[3,2]$	29286	0	$[3,2]$	29286
	$[2,3]$	4772		$[2,3]$	4772		$[2,3]$	4772
	$x^1=[1,2]$	166		$x^1=[1,2]$	166		$x^1=[1,2]$	166
	$[2,1]$	4176	1	$[2,2]$	4401	1	$x^2=[0,2]$	81
1	$[2,2]$	4401		$[1,3]$	262	2	$[-1,2]$	2646
	$[1,3]$	262		$x^2=[0,2]$	81		$[0,3]$	152
	$x^2=[0,2]$	81	2	$[1,2]$	166		$[1,2]$	166
	$[1,1]$	106		$[0,3]$	152		$x^3=[0,1]$	36
2	$[1,2]$	166		$[-1,2]$	2646	3	$x^4=[0,0]$	17
	$[0,3]$	152		$x^3=[0,1]$	36	4	$[0,-1]$	24
	$[-1,2]$	2646	3	$[1,1]$	106		$[0,1]$	36
	$x^3=[0,1]$	36		$[0,2]$	81		$[1,0]$	82
3	$[1,1]$	106		$[-1,1]$	2466		$[-1,0]$	2402
	$[0,2]$	81		$x^4=[0,0]$	17	5	$[0,-0.5]$	17.25
	$[-1,1]$	2466	4	$[1,0]$	82		$[0,0.5]$	23.25
	$x^4=[0,0]$	17		$[0,1]$	36		$x^6=[0.5,0]$	1.0625
4	$[1,0]$	82		$[-1,0]$	2402	6	$[1,0]$	82
	$[0,1]$	36		$[0,-1]$	24		$x^7=[0.5,-0.5]$	0.375
	$[-1,0]$	2402	5	$x^6=[0.5,0]$	1.0625	7	$[0.5,-1]$	4.3125
	$[0,-1]$	24	6	$[1,0]$	82		$[1,-0.5]$	83.5
Incumbent solutions after a total of 100 function evaluations								
	$[0.398,-0.332]$	2.2×10^{-5}		$[0.3999,-0.3330]$	9.8×10^{-7}		$[0.4000,-0.3334]$	1.7×10^{-8}

CS evolution

1961 Hooke and Jeeves - Pattern Search
1997 Torczon - Genaralized Pattern Search



Mesh coarsens on successful iterations

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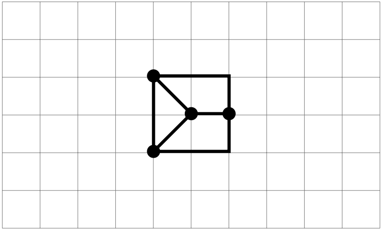

Mesh refines on unsuccessful iterations

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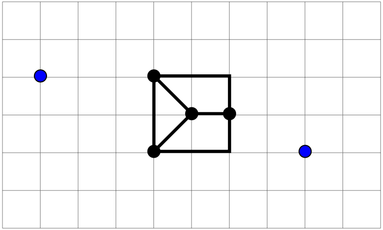

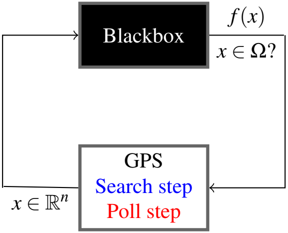

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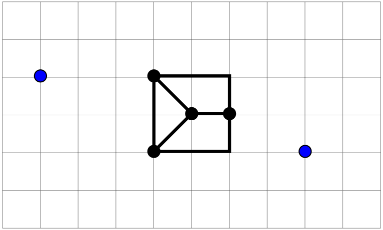
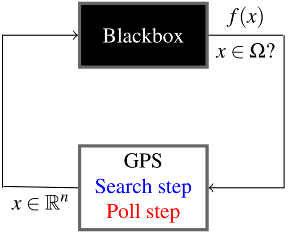




Theorm (Convergence analysis 2003 - Clark calculus)

Let $\hat{x}$ be an accumlation point of the sequence of mesh local optimizers on meshes that get infinitely fine.
If f is Lipshitz near $\hat{x}$, then $f^{\circ}(\hat{x};d) \geq 0$ for all directions d used infinitely often.
The set of such directions forms a positive basis for $\mathbb{R}^n$

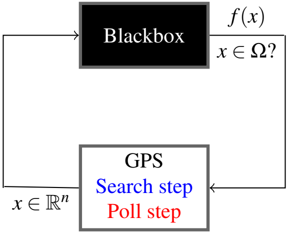
[0] Initializations (x_0, Δ_0)

[1] Iteration k

- **[1.1] (global) Search**
  - select a finite number of mesh points
  - sort these points
  - evaluate candidates opportunistically
- **[1.2] (local) Poll** (if the Search failed)
  - construct poll set $P_k = \{x_k + \Delta_k d : d \in D_k\}$
  - sort(P_k)
  - evaluate candidates opportunistically

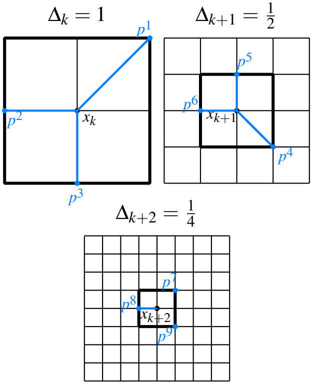
[2] Updates

- if success
  - $x_{k+1} \leftarrow$ success point
  - possibly increase Δ_k
- else
  - $x_{k+1} \leftarrow x_k$
  - decrease Δ_k
- $k \leftarrow k+1$, stop or go to **[1]**



GPS: Example of poll directions

$P_k = \{x_k + \Delta_k d : d \in D_k\}$; $n+1$ mesh points at distance Δ_k from x_k



14 different ways of defining D_k on this mesh

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The MADS algorithm

MADS main algorithm

1: Initialization
 $x^0 \in \mathbb{R}^n$ initial point
 $\Delta^0 \in (0, \infty)$ initial frame size parameter

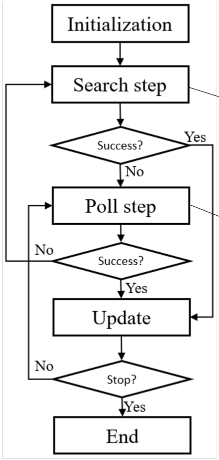
2: Parameter Update
 set the mesh size parameter to $\delta^k \leq \Delta^k$
 define the mesh M^k

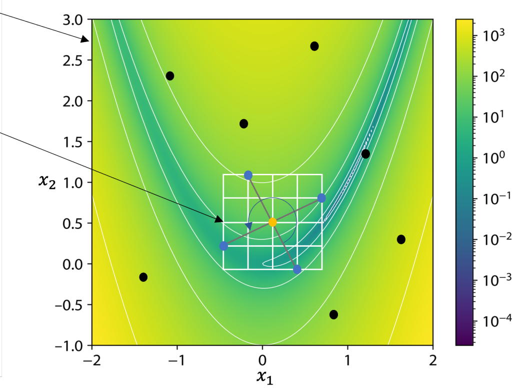
3: "Optional" global Search on mesh M^k
 if $f(t) < f(x^k)$ for some t in a finite subset of the mesh M^k
  set $x^{k+1} \leftarrow t$ and $\Delta^{k+1} \leftarrow 2\Delta^k$ and go to Step 5.

4: Local Poll on Mesh M^k
 select a positive spanning set D^k_Δ
 if $f(t) < f(x^k)$ for some $t \in P^k = \{x^k + \delta^k d : d \in D^k_\Delta\}$ in a finite subset of the mesh M^k
  set $x^{k+1} \leftarrow t$ and $\Delta^{k+1} \leftarrow 2\Delta^k$
 else set $x^{k+1} \leftarrow x^k$ and $\Delta^{k+1} \leftarrow \frac{1}{2}\Delta^k$

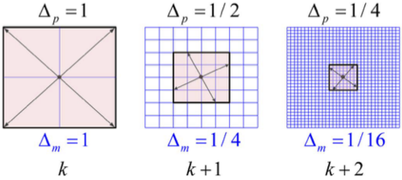
5: Termination check
 otherwise $k \leftarrow k+1$ and return to Step 2.

MADS algorithm workflow





Mesh and frame definitions



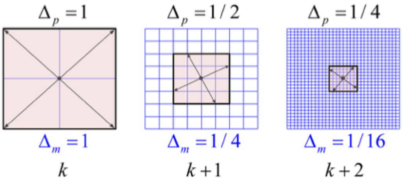
Definition: Mesh and Mesh Size Parameter

Let $G \in \mathbb{R}^{n \times n}$ be an invertible matrix and the columns of $Z \in \mathbb{Z}^{n \times p}$ form a positive spanning set for $\mathbb{R}^n$. Define $D = GZ$. The mesh of coarseness $\delta^k > 0$ generated by D, centered at the incumbent solution $x_k \in \mathbb{R}^n$, is defined by $M^k := \{x^k + \delta^k D_y : y \in \mathbb{N}^p \subset \mathbb{R}^n, \}$ where δ^k is called the mesh size parameter.

Definition: Frame and Frame Size Parameter

Let $G \in \mathbb{R}^{n \times n}$ be an invertible matrix and the columns of $Z \in \mathbb{Z}^{n \times p}$ form a positive spanning set for $\mathbb{R}^n$. Define $D = GZ$. Select a mesh size parameter $\delta^k > 0$ and let Δ^k be such that $\delta^k \leq \Delta^k$. The frame of extent Δ^k generated by D, centered at the incumbent solution $x_k \in \mathbb{R}^n$, is defined by $F^k := \{x \in M^k : ||x - x^k||_\infty \leq \Delta^k b\}$ with $b = max\{||d'||_\infty : d' \in \mathbb{D}\}$ and Δ^k is called the frame size parameter.

Dense (rich) set of polling directions



Definition: Asymptotically Dense

The set $V \subseteq \mathbb{R}^n$ is said to be asymptotically dense if the normalised set $\{v/||v|| : v \in V\}$ is dense on the unit sphere $S = \{w \in \mathbb{R}^n : |w| = 1\}$.

Definition: Householder Matrix

Let $V \subseteq \mathbb{R}^n$ be a normalized vector. The Householder matrix H associated with v is $H := I - 2vv^T \in \mathbb{R}^{n \times n}$, where I is the $n \times n$ identity matrix.

- What is blackbox optimization?
- Functions differentiability
- Direct search methods
- Mesh adaptive direct search method
- Implementations
- Running example

MADS implementations (1/2)

- MADS is a general framework. It defines the conditions on the directions, but do not define the direction themselves
- There are several implementations:
  - LT-MADS: Based on Lower-Triangular random matrices
  - QR-MADS: Based on the QR decomposition and on normally distributed directions
  - OrthoMADS: Quasi-random, deterministic, and orthogonal directions. Current default in NOMAD

MADS implementations (2/2)

- Several programs that implement MADS are available:
  - MATLAB: `NOMADm`: https://github.com/khbalhandawi/MECH559_notebooks/blob/master/MATLAB_Algorithms/NomadM/nomadm.m
  - Python: `OMADS`: https://ahmed-bayoumy.github.io/OMADS/
  - C++ (with interfaces to various languages): `NOMAD`: https://nomad-4-user-guide.readthedocs.io/en/latest/index.html
    This implements the state-of-the-art in MADS development.

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