Direct Search methods

MTH8418

S. Le Digabel, Polytechnique Montréal

Winter 2020

(v3)

Plan

Blackbox optimization problems

- We consider the optimization problem

$$\min_{x \in \Omega} \quad f(x)$$

  where the evaluations of f and the functions defining Ω are usually the result of a computer code (a blackbox)

- Extreme Barrier approach: We focus on the optimization of f_Ω instead of f, with $f_\Omega(x) = \begin{cases} f(x) \text{ if } x \in \Omega \\ \infty \text{ otherwise} \end{cases}$

- Better treatments of constraints are studied in Lesson #9

Introduction

- Generalized Pattern Search (GPS) [Torczon, 1997]
- Generalization of the CS and H&J methods
- Mesh at iteration k:

$$M_k = \bigcup_{x \in V_k} \{x + \Delta_k D z : z \in \mathbb{N}^{n_D}\}$$

- Mesh size parameter: $\Delta_k \in \mathbb{R}^+$
- Cache: Set V_k of the points already evaluated by the start of iteration k
- Directions:
  - Matrix D of dimension $n \times n_D$
  - One column in D = One direction in $\mathbb{R}^n$
  - Typically D is taken as $[I_n \;\; -I_n]$ (as in CS)

[0] Initializations (x_0, Δ_0)

[1] Iteration k

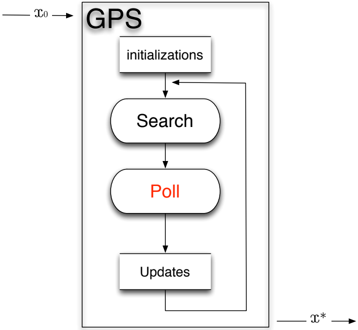
- **[1.1] (global) Search**
  - select a finite number of mesh points
  - sort these points
  - evaluate candidates opportunistically
- **[1.2] (local) Poll** (if the Search failed)
  - construct poll set $P_k = \{x_k + \Delta_k d : d \in D_k\}$
  - sort(P_k)
  - evaluate candidates opportunistically

[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]**

The Poll (1/2)

- Poll set:
  $P_k = \{x_k + \Delta_k d : d \in D_k\}$ where x_k is the current incumbent, or the poll center
- Poll directions: A positive spanning set $D_k \subset \mathbb{R}^n$ where each direction $d \in D_k$ is one of the directions of D
- The directions correspond typically to a minimal positive basis ($n+1$ directions) or a maximal positive basis ($2n$ directions)

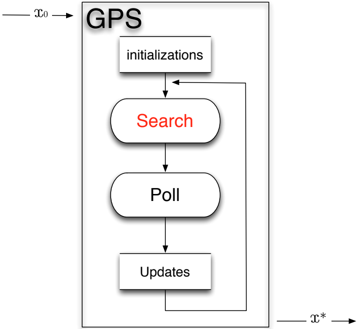


The Poll (2/2)

- The trial points in P_k are evaluated following the opportunistic strategy: evaluations are interrupted as soon as a new better solution is found
- Trial points ordering is then crucial in practice. It can be based on:
  - Model or surrogate values
  - Angle with the gradient of a model
  - Angle with the last direction of success
  - etc.

The Search

- Flexible and global search strategy
- Is executed prior to the poll step
- Is valid for a finite number of mesh points
- Users can define their own strategy, specific to their problem
- Generic strategies exist (random, LH, speculative, etc.)



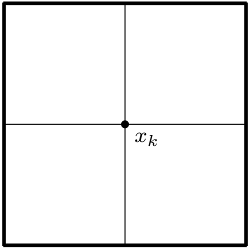
Mesh size update

- Update $\Delta_{k+1} \leftarrow \tau^{\omega}\Delta_k$ with $\tau > 1$ rational and $\omega \in \{\omega^-, \omega^+\}$, with ω^- integer ≤ -1, ω^+ integer ≥ 0
- CS: $\tau = 2$, $\omega^+ = 0$, $\omega^- = -1$
- GPS default: $\tau = 2$, $\omega^+ = 1$, $\omega^- = -1$

Coordinate Search (CS): Polling directions

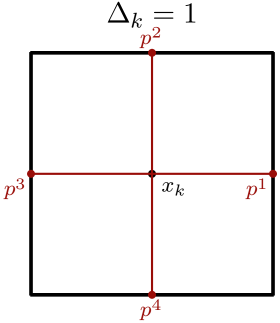
$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k

$\Delta_k = 1$



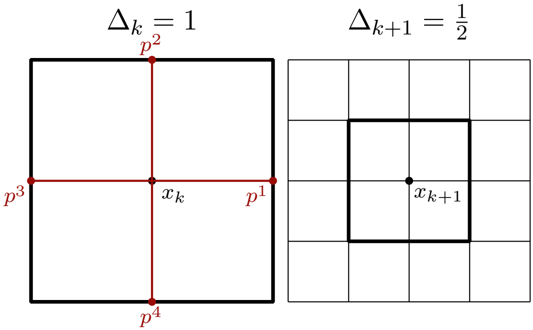
Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k



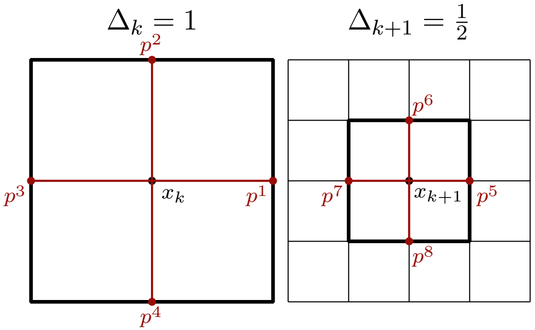
Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k



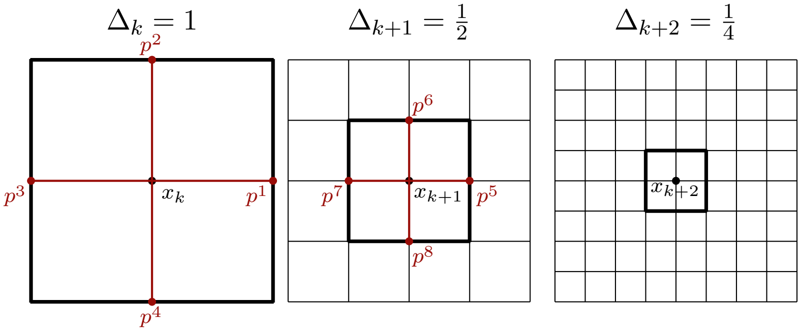
Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k



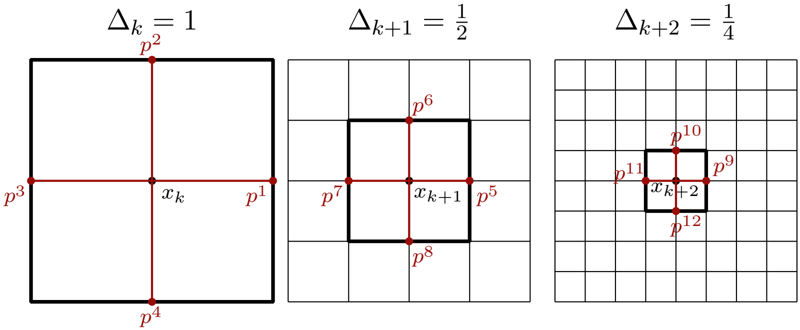
Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k



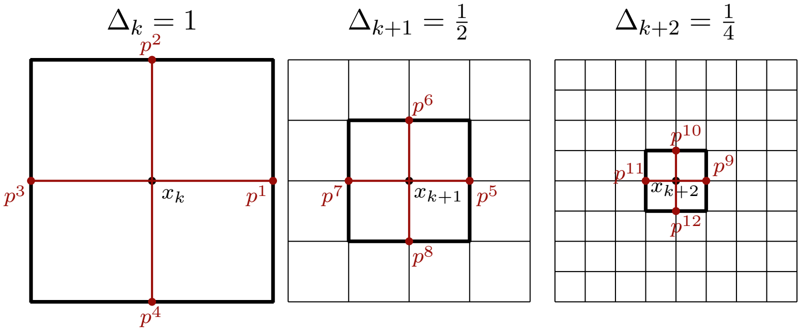
Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k



Coordinate Search (CS): Polling directions

$P_k = \{x_k \pm \Delta_k e_i\}$; $2n$ mesh points at distance Δ_k from x_k

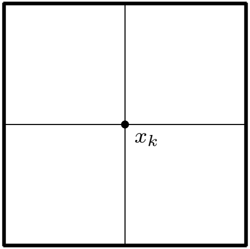


Always the same $2n = 4$ directions

GPS: Example of poll directions

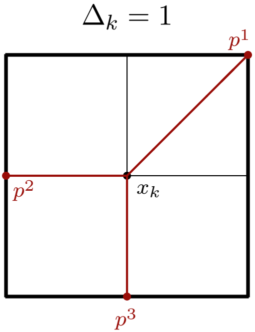
$P_k = \{x_k + \Delta_k d : d \in D_k\}$; $n+1$ mesh points at distance Δ_k from x_k

$\Delta_k = 1$



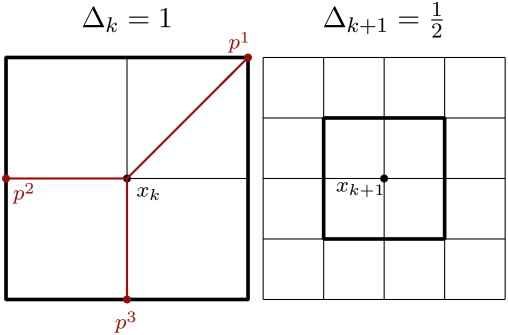
GPS: Example of poll directions

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



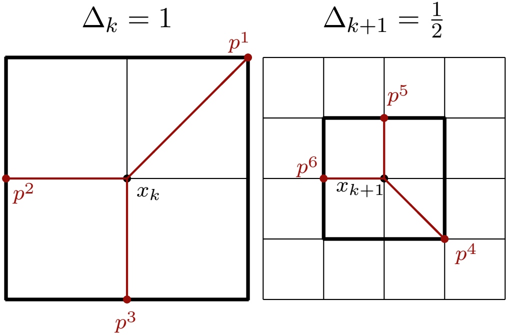
GPS: Example of poll directions

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



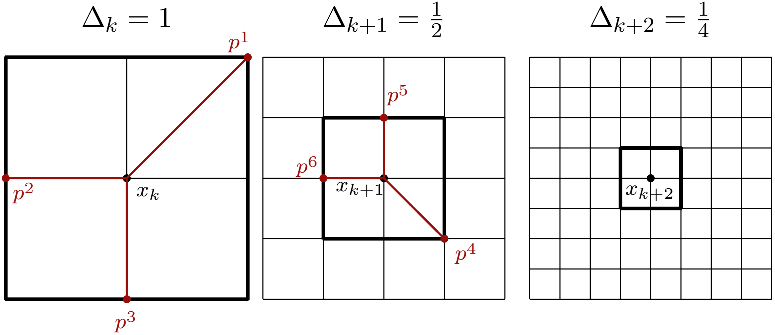
GPS: Example of poll directions

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



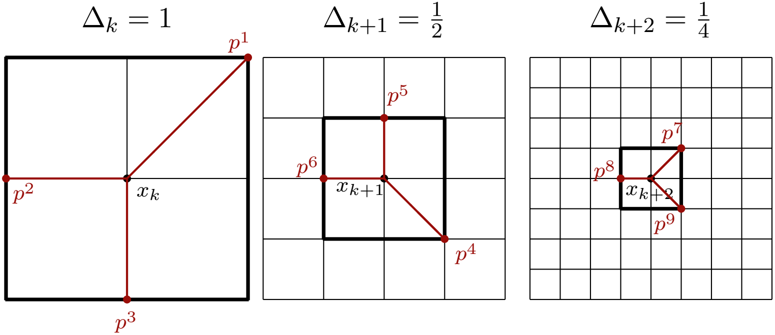
GPS: Example of poll directions

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



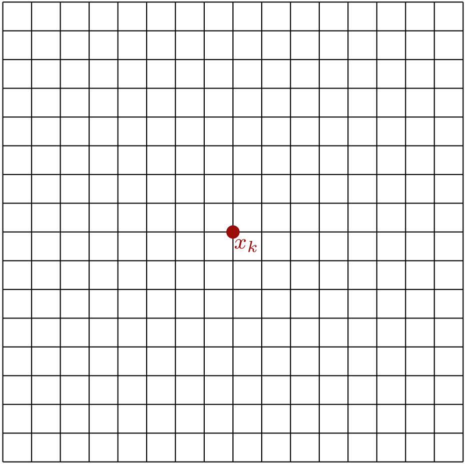
GPS: Example of poll directions

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



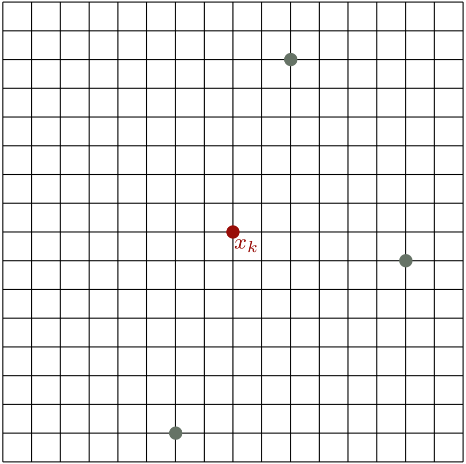
14 different ways of defining D_k on this mesh

GPS: Poll and Search

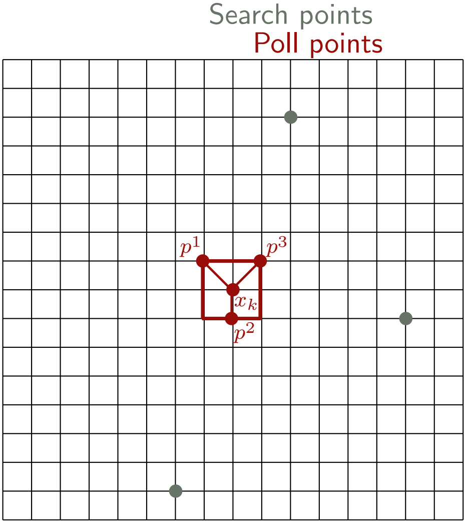


GPS: Poll and Search

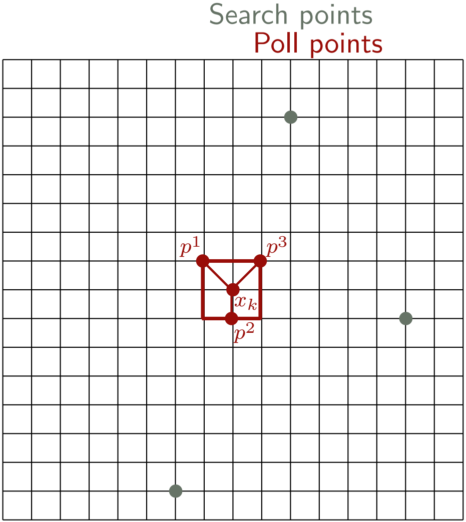
Search points

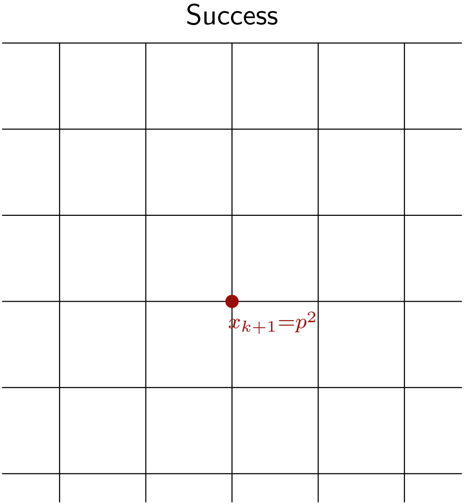


GPS: Poll and Search

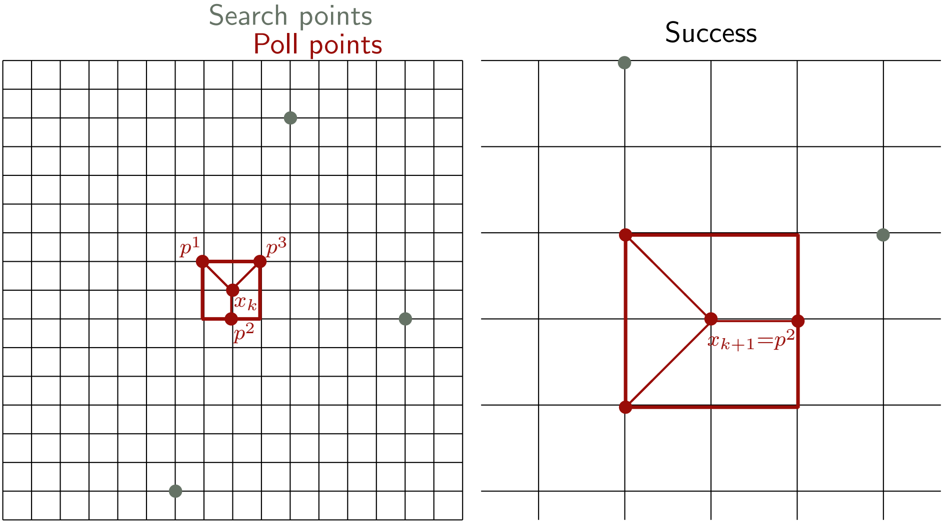


GPS: Poll and Search

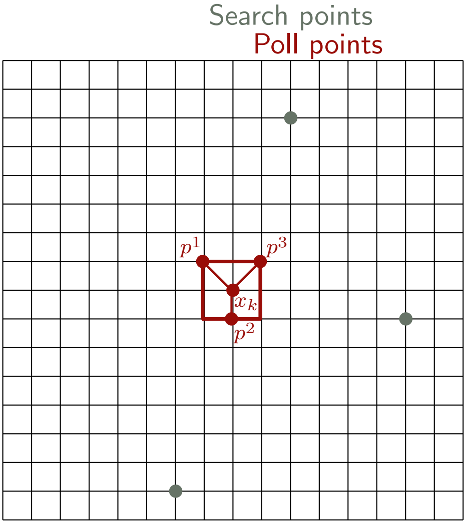


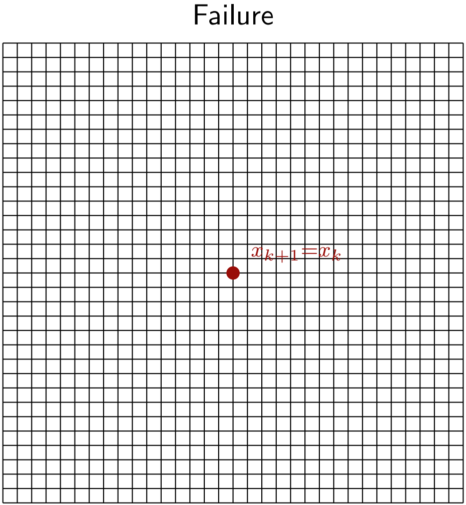


GPS: Poll and Search

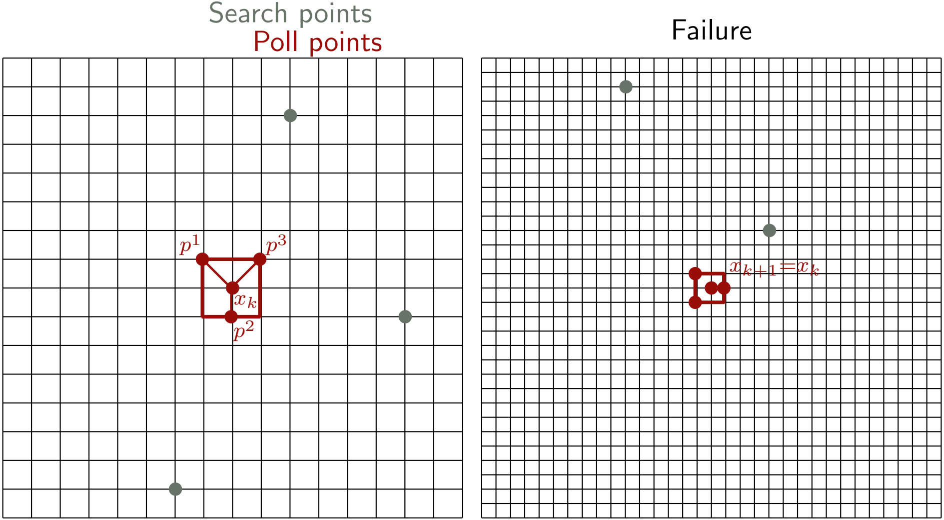


GPS: Poll and Search





GPS: Poll and Search



Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_{k} \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_k \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Theorem

If f Lipschitz near $\hat{x}$, then $f^\circ(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times

Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_k \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Theorem

If f Lipschitz near $\hat{x}$, then $f^\circ(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times

PROOF: $$f^\circ(\hat{x}; d) := \limsup_{y \to \hat{x},\ t \downarrow 0} \frac{f(y + td) - f(y)}{t}$$

Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_k \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Theorem

If f Lipschitz near $\hat{x}$, then $f^\circ(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times

PROOF:

$$f^\circ(\hat{x}; d) := \limsup_{y \to \hat{x},\ t \downarrow 0} \frac{f(y + td) - f(y)}{t} \geq \limsup_{k \in K} \frac{f(x_k + \Delta_k d) - f(x_k)}{\Delta_k}$$

Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_k \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Theorem

If f Lipschitz near $\hat{x}$, then $f^\circ(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times

PROOF:
$$\begin{aligned} f^\circ(\hat{x}; d) &:= \limsup_{y \to \hat{x},\ t \downarrow 0} \frac{f(y + td) - f(y)}{t} \\ &\geq \limsup_{k \in K} \frac{f(x_k + \Delta_k d) - f(x_k)}{\Delta_k} \geq 0 \end{aligned}$$

Note: These directions form a positive spanning set

Convergence analysis

If the series of iterates $\{x_k\}$ belongs to a bounded set, then

- $\lim_k \Delta_k = 0$ for any infinite subset of indices
- There exists $\hat{x} \in \mathbb{R}^n$ the limit of a subsequence of mesh local minimizers for meshes that get infinitely fine: $x_k \to \hat{x}$, with $f(x_k + \Delta_k d) \geq f(x_k)$ for all $d \in D_k$, and $k \in K$

Theorem

- *If f Lipschitz near $\hat{x}$, then $f^\circ(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times*
- *If f regular near $\hat{x}$, then $f'(\hat{x}; d) \geq 0$ for all directions $d \in D$ used infinitely many times*
- *If f strictly differentiable near $\hat{x}$, then $\nabla f(\hat{x}) = 0$*

Limitations

- In order to move from a non-optimal point, the poll step has to generate descent directions inside the tangent cone
- With general constraints, it is impossible to identify all the tangent cone generators
- The biggest limitation is then the fixed and limited number of possible directions

Generalized Pattern Search (GPS)

Mesh Adaptive Direct Search (MADS)

Other direct-search methods

References

The MADS acronyms

- **MADS** (**M**esh **A**daptive **D**irect **S**earch)
  $\rightarrow$ The algorithmic framework without the definition of the polling directions
- **LT-MADS**: Original MADS implementation
- **OrthoMADS**: Second MADS implementation
- **QR-MADS**: Van Dyke and Asaki MADS implementation
- `NOMAD` (**N**onlinear **O**ptimization with the **MAD**S algorithm):
  $\rightarrow$ The software package. Includes LT-MADS and OrthoMADS
- NOMADS does not exist

Mesh Adaptive Direct Search (MADS)

- [Audet and Dennis, Jr., 2006]
- Generalization of GPS
- Better convergence result: If f Lipschitz near $\hat{x}$, it is a Clarke stationary point:

$$f^\circ(\hat{x}; d) \geq 0 \text{ for all } d \in T_\Omega^{Cl}(\hat{x})$$

(T_Ω^{Cl} is a generalization of the tangent cone)

Directions

- The directions $D_k \subset \mathbb{R}^n$ are not taken in D. But each direction $d \in D_k$ can be written as a nonnegative integer combination of directions of D
- The set of normalized directions grows dense in the unit sphere, i.e.:

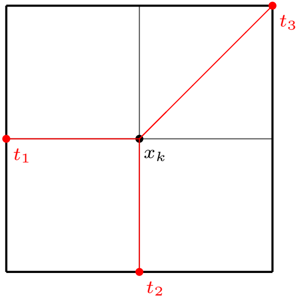
  For all $\varepsilon > 0$, and for all $d \in \mathbb{R}^n$, there exists one MADS direction d_k such that $\left\| \frac{d_k}{\|d_k\|} - \frac{d}{\|d\|} \right\| < \varepsilon$

Mesh

- The GPS mesh size parameter Δ_k is replaced by the MADS mesh size parameter Δ_k^m, and the new poll size parameter Δ_k^p is introduced
- The mesh and the poll set remain the same with $M_k = \bigcup_{x \in V_k} \{x + \Delta_k^m D z : z \in \mathbb{N}^{n_D}\}$ and $P_k = \{x_k + \Delta_k^m d : d \in D_k\}$, but now we have $\|\Delta_k^m d\| \simeq \Delta_k^p$
- $\Delta_k^m \leq \Delta_k^p$ at each iteration k, and Δ_k^m is reduced faster than Δ_k^p
- Typically:
  - $\Delta_{k+1}^m \leftarrow 4\Delta_k^m$ or $\Delta_k^m/4$
  - $\Delta_{k+1}^p \leftarrow 2\Delta_k^p$ or $\Delta_k^p/2$
  - $\Delta_k^p = \sqrt{\Delta_k^m}$, with $\Delta_k^m, \Delta_k^p \leq 1$

Poll illustration (successive fails and mesh shrinks)

$$\Delta_k^m = \Delta_k^p = 1$$

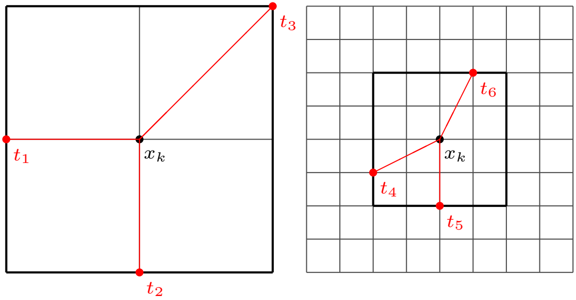


poll trial points=$\{t_1, t_2, t_3\}$

Poll illustration (successive fails and mesh shrinks)

$\Delta_k^m = \Delta_k^p = 1$

$\Delta_{k+1}^m = 1/4$
$\Delta_{k+1}^p = 1/2$



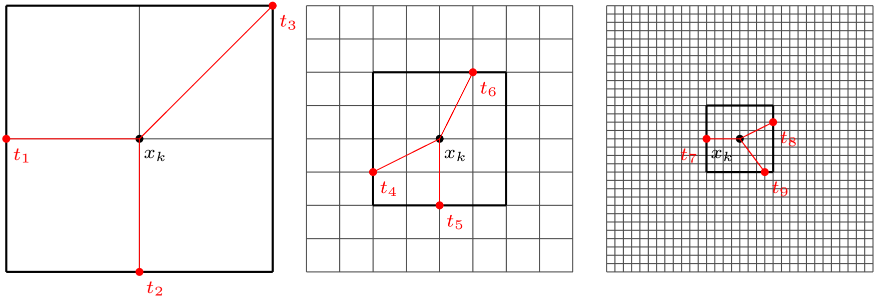
poll trial points$=\{t_1, t_2, t_3\}$ $= \{t_4, t_5, t_6\}$

Poll illustration (successive fails and mesh shrinks)

$\Delta_k^m = \Delta_k^p = 1$

$\Delta_{k+1}^m = 1/4$
$\Delta_{k+1}^p = 1/2$

$\Delta_{k+2}^m = 1/16$
$\Delta_{k+2}^p = 1/4$

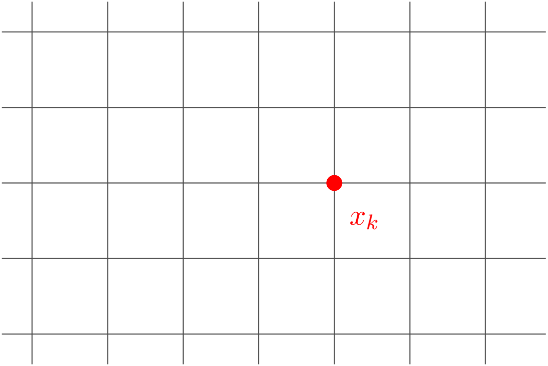


poll trial points$=\{t_1, t_2, t_3\}$ $=\{t_4, t_5, t_6\}$ $=\{t_7, t_8, t_9\}$

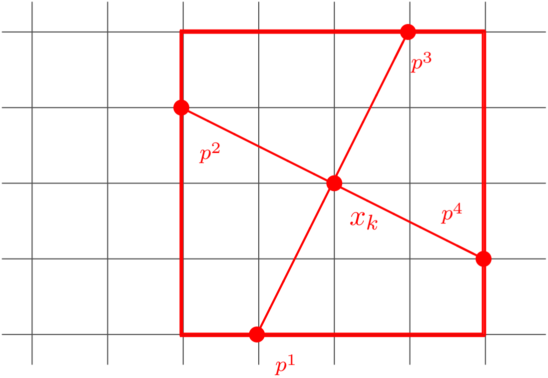
MADS implementations

- 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 [Audet and Dennis, Jr., 2006]
  - QR-MADS: Based on the QR decomposition and on normally distributed directions [Van Dyke and Asaki, 2013]
  - OrthoMADS: Quasi-random, deterministic, and orthogonal directions. Current default in `NOMAD` [Abramson et al., 2009]

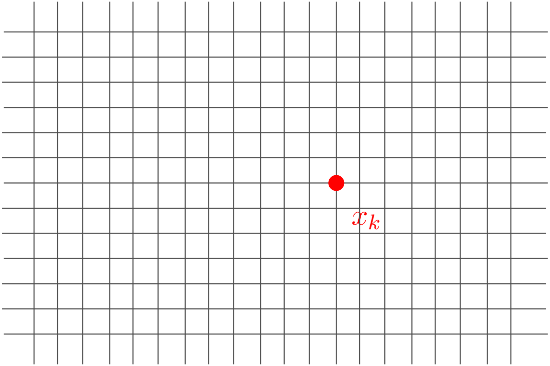
OrthoMADS



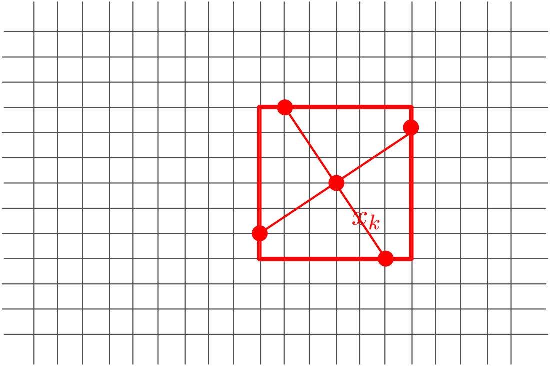
OrthoMADS



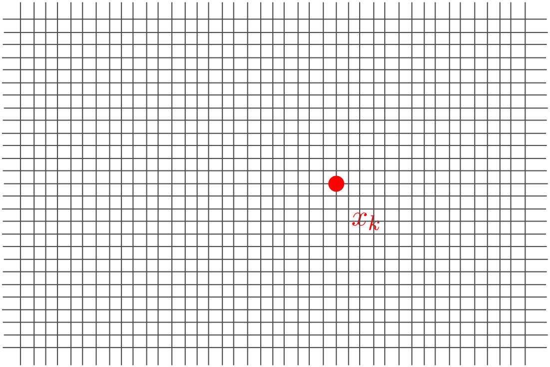
OrthoMADS



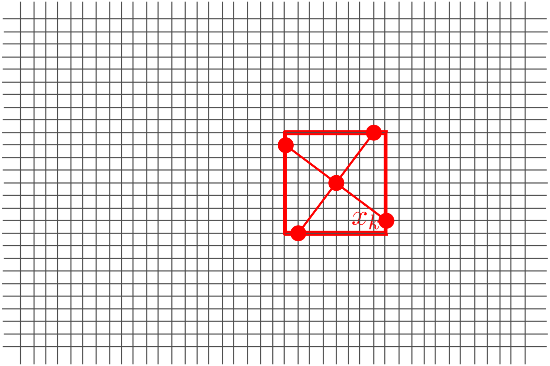
OrthoMADS



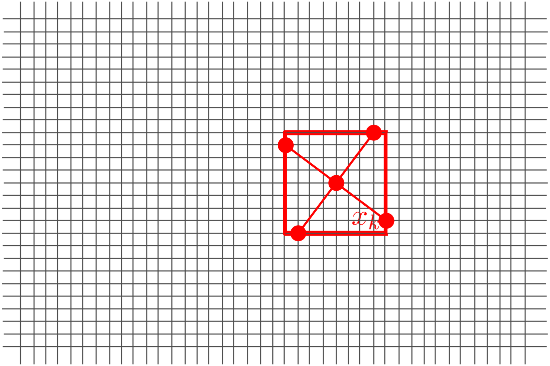
OrthoMADS



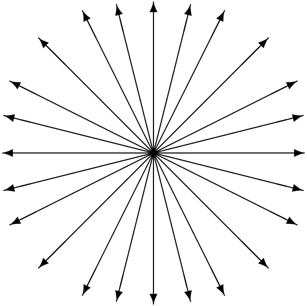
OrthoMADS



OrthoMADS

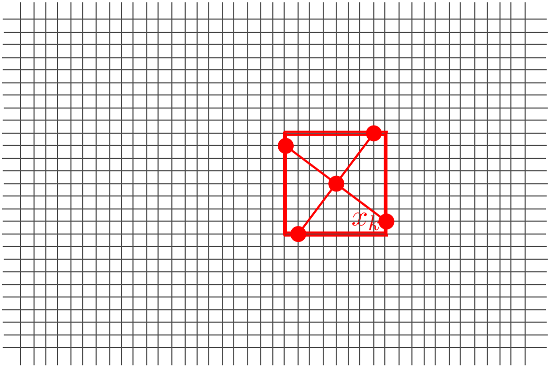


Set of normalized directions is dense in the unit sphere

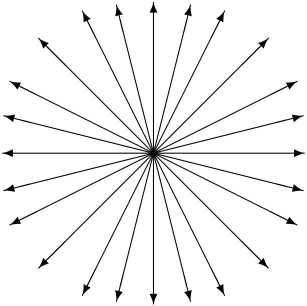


infinite number of directions

OrthoMADS



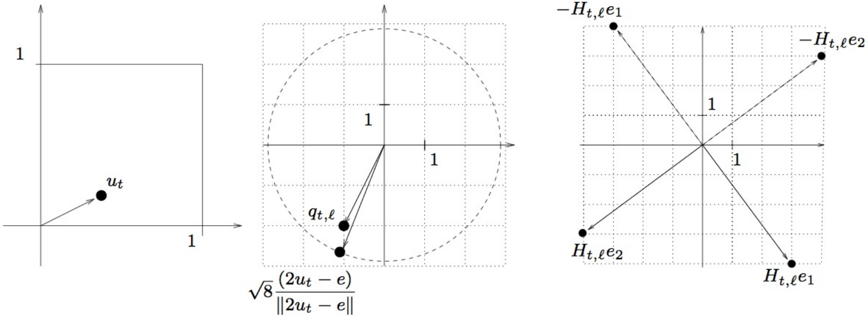
Set of normalized directions is dense in the unit sphere



infinite number of directions

- OrthoMADS is deterministic
- At each iteration, directions are orthogonal

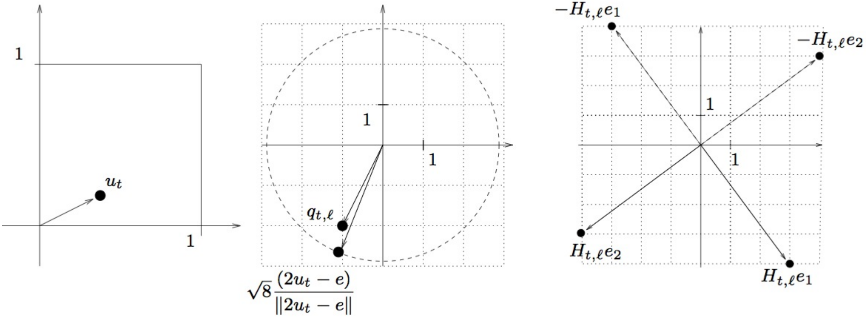
- OrthoMADS is based on the quasi-random Halton sequence [Halton, 1960] in order to generate a sequence of vectors $\{u_t\}_{t=1}^{\infty}$ dense in $[0;1]^n$
- u_t is transformed into $\frac{2u_t - e}{\|2u_t - e\|}$ on the unit sphere, with $e = (1, 1, \ldots, 1)$, and scaled
- The latter is projected to the current mesh ($\rightarrow q_{t,\ell}$)



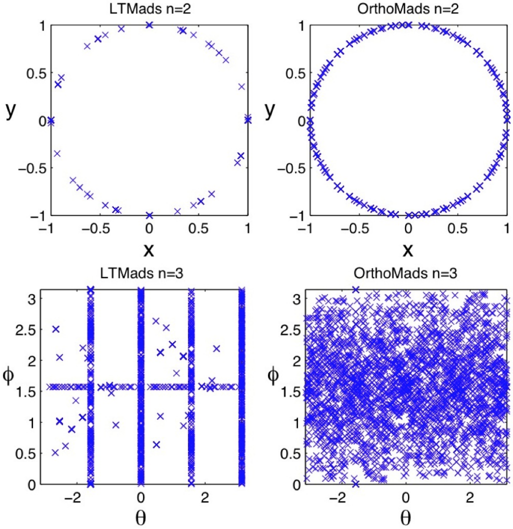
- The Householder transformation is applied:

$$H = \|q_{t,\ell}\|^2 I_n - 2q_{t,\ell}q_{t,\ell}^\top$$

- By construction, H is an integer orthogonal basis of $\mathbb{R}^n$
- The poll directions are the columns of H and $-H$



OrthoMADS: Dense directions



OrthoMADS $n+1$

- [Audet et al., 2014]
- For various reasons, OrthoMADS is preferred to LT-MADS. LT-MADS defines $n+1$ and $2n$ types of directions, and OrthoMADS had only the $2n$ variant

	LT-MADS	OrthoMADS
$n+1$	2006	2014
$2n$	2006	2009

- Some tests suggested that the LT-MADS implementation was more efficient with $n+1$ directions
- This more recent OrthoMADS variant uses $n+1$ directions as well

General framework #1

Idea: Given a poll set of $2n$ trial points, prune it to n points and add a direction to obtain $n+1$ points

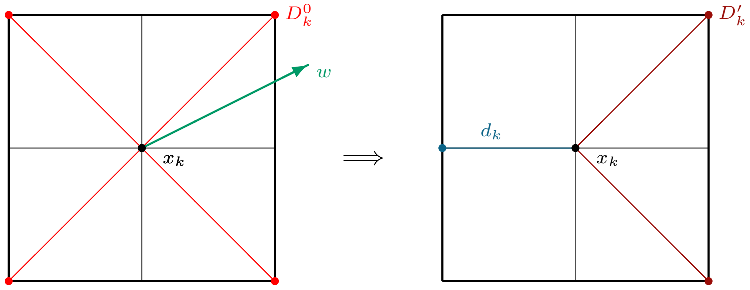
Poll at iteration k

$P_k^o = \{x_k + \Delta_k d : d \in D_k^o\}$ (original poll set)
extract $D_k' \subset D_k^o$
compute new direction d_k
$D_k = D_k' \cup \{d_k\}$
construct $P_k = \{x_k + \Delta_k d : d \in D_k\}$ (reduced poll set)
sort(P_k)
evaluate(P_k) (opportunistically)

OrthoMads $n+1$ with framework #1

- $D_k^o = [H_k \;\; -H_k]$ is the original OrthoMADS spanning set with $2n$ directions and $H_k \in \mathbb{Z}^{n \times n}$ an orthogonal basis with integer coefficients
- The selection of n columns of D_k^o to obtain D_k' is based on a target direction $w \in \mathbb{R}^n$
- The target direction is taken as the last direction of success
- The $(n+1)^{\text{th}}$ direction is $d_k = -\sum_{d \in D_k'} d$

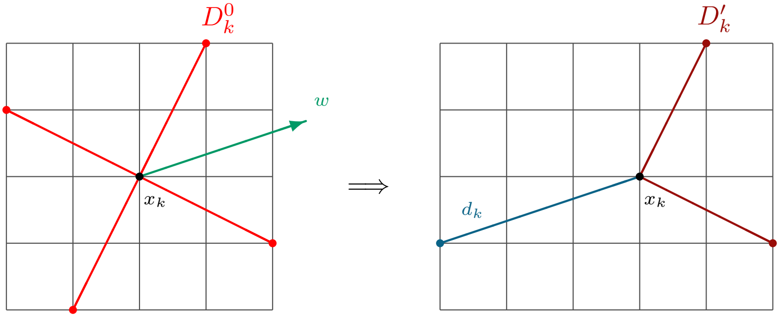
OrthoMads $n+1$ with framework #1: Idea



$2n$ directions D_k^0

$n+1$ directions $D_k = D'_k \cup \{d_k\}$

OrthoMads $n + 1$ with framework #1: Idea



$2n$ directions D_k^0

$n + 1$ directions $D_k = D_k' \cup \{d_k\}$

Completion using function values

- Second and more general framework
- This version is not limited to OrthoMADS and may be applied to any poll sets. For example hybrid versions with more than $2n$ points
- The first framework is decomposed allowing to evaluate n trial points in a first step and possibly one last $(n+1)^{\text{th}}$ point $y_k = x_k + d_k \Delta_k$
- y_k is constructed by exploiting the function values at the first n points
- y_k must lie on the mesh and d_k must be inside the cone of the negative directions of D'_k so that the poll directions remain a positive spanning set

General framework #2

Poll at iteration k

- $P_k^o = \{x_k + \Delta_k d : d \in D_k^o\}$ (original poll set)
- extract $D_k' \subset D_k^o$ and construct P_k'
- sort (P_k')
- evaluate (P_k') (opportunistically)
- Success
  - interrupt iteration
- Failure
  - compute new direction d_k
  - evaluate $(x_k + \Delta_k d_k)$

Use of quadratic models

Quadratic models may be used at two different levels:

1. In Framework #1: The simplex gradient is taken as the target direction w
2. In Framework #2: Optimize a model to determine the last trial point $y_k = x_k + \Delta_k d_k$

Generalized Pattern Search (GPS)

Mesh Adaptive Direct Search (MADS)

Other direct-search methods

References

Other direct-search methods (1/2)

- **Hooke and Jeeves:**
  - [Hooke and Jeeves, 1961]
  - Original Pattern Search method
  - CS directions
  - Precursor of the Search step: "Exploratory moves"
  - Introduced the term "Direct-Search"
- **Implicit filtering:**
  - [Winslow et al., 1991]
  - Simplex gradients using second-order approximations
  - Line search
  - Quasi-Newton update
  - IFFCO, IMFIL software packages

Other direct-search methods (2/2)

- **DIRECT:**
  - [Jones et al., 1993]
  - **DI**viding **RECT**angles
  - Global optimization
  - The space is divided into hyperrectangles, and the most promising ones are divided again into smaller hyperrectangles
  - The blackbox is evaluated at the center of the hyperrectangles
  - DIRECT software
- **GSS:**
  - [Kolda et al., 2003]
  - **G**enerating **S**et **S**earch
  - GPS with Search and Poll steps
  - Additional directions conforming to bounds and linear constraints
  - HOPSPACK software

Generalized Pattern Search (GPS)

Mesh Adaptive Direct Search (MADS)

Other direct-search methods

References

References I

Abramson, M., Audet, C., Dennis, Jr., J., and Le Digabel, S. (2009).
OrthoMADS: A Deterministic MADS Instance with Orthogonal Directions.
SIAM Journal on Optimization, 20(2):948–966.

Audet, C. and Dennis, Jr., J. (2006).
Mesh adaptive direct search algorithms for constrained optimization.
SIAM Journal on Optimization, 17(1):188–217.
(MADS).

Audet, C., Ianni, A., Le Digabel, S., and Tribes, C. (2014).
Reducing the Number of Function Evaluations in Mesh Adaptive Direct Search Algorithms.
SIAM Journal on Optimization, 24(2):621–642.
(OrthoMADS $n + 1$).

Halton, J. (1960).
On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals.
Numerische Mathematik, 2(1):84–90.
(Halton sequence).

References II

Hooke, R. and Jeeves, T. (1961).
"Direct Search" Solution of Numerical and Statistical Problems.
Journal of the Association for Computing Machinery, 8(2):212–229.
(H&J algorithm).

Jones, D., Perttunen, C., and Stuckman, B. (1993).
Lipschitzian optimization without the Lipschitz constant.
Journal of Optimization Theory and Application, 79(1):157–181.
(DIRECT).

Kolda, T., Lewis, R., and Torczon, V. (2003).
Optimization by direct search: New perspectives on some classical and modern methods.
SIAM Review, 45(3):385–482.
(GSS).

Torczon, V. (1997).
On the convergence of pattern search algorithms.
SIAM Journal on Optimization, 7(1):1–25.
(GPS).

References III

Van Dyke, B. and Asaki, T. (2013).
Using QR Decomposition to Obtain a New Instance of Mesh Adaptive Direct Search with Uniformly Distributed Polling Directions.
Journal of Optimization Theory and Applications, 159(3):805–821.
(QR-MADS).

Winslow, T., Trew, R., Gilmore, P., and Kelley, C. (1991).
Doping profiles for optimum class B performance of GaAs MESFET amplifiers.
In *Proceedings IEEE/Cornell Conference on Advanced Concepts in High Speed Devices and Circuits*, pages 188–197.
(Implicit Filtering).