NOMAD User Guide
Version 3.8.0

Sébastien Le Digabel,
Christophe Tribes and
Charles Audet

How to use this guide:

- A general introduction of NOMAD is presented in Chapter 1.

- New users of NOMAD:
  Chapter 2 describes how to install the software application.
  Chapter 3 describes how to get started with NOMAD.

- NOMAD utilization:
  All users can find in Chapters 4 to 7 ways to tailor problem definition, algorithmic settings and software output.

- Tricks that may help solving specific problems are presented in Chapter 5.

Please cite NOMAD with references [23, 44].

List of acronyms

NOMAD	Nonlinear Optimization by Mesh Adaptive Direct Search (software)
MADS	Mesh Adaptive Direct Search (algorithm)
LT-MADS	Original MADS
OrthoMADS	Second MADS
BiMADS	Bi-objective MADS algorithm
p-MADS	Parallel version of MADS
Coop-MADS	Parallel version of MADS with cooperation
SGTELIB	Surrogate library for NOMAD
PSD-MADS	Parallel version of MADS with space decomposition
VNS	Variable Neighborhood Search
GPS	Generalized Pattern Search

Contents

Contents

Preface

In many situations, one is interested in identifying the values of a set of variables that maximize or minimize some objective function. Furthermore, the variables cannot take arbitrary values, as they are confined to an admissible region and need to satisfy some prescribed requirements. NOMAD is a software application designed to solve these kind of problems.

The nature of the objective function and constraints dictates the type of optimization methods that should be used to tackle a given problem. If the optimization problem is convex, or if the functions are smooth and easy to evaluate, or if the number of variables is large, then NOMAD is not the solution that you should use. NOMAD is intended for time-consuming blackbox simulation with a small number of variables. NOMAD is often useful when other optimizers fail.

These nasty problems are called *blackbox optimization problems*. With NOMAD some constraints may be evaluated prior to launching the simulation, and others may only be evaluated *a posteriori*. The simulations may take several seconds, minutes, hours or even days to compute. The blackbox can have limited precision and be contaminated with numerical noise. It may also fail to return a valid output, even when the input appears acceptable. Launching twice the simulation from the same input may produce different outputs. These unreliable properties are frequently encountered when dealing with real problems. The term blackbox is used to indicate that the internal structure of the target problem, such as derivatives or their approximations, cannot be exploited as it may be unknown, hidden, unreliable or inexistent. There are situations where some structure such as bounds may be exploited and in some cases, a surrogate of the problem may be supplied to NOMAD or a model may be constructed and trusted.

This document describes how to use NOMAD to solve your blackbox optimization problem.

Part I

FIRST NOMAD STEPS

Chapter 1

Introduction

1.1 What is NOMAD?

> NOMAD = **N**onlinear **O**ptimization by **M**esh **A**daptive **D**irect Search

NOMAD is a software application for simulation-based optimization. It can efficiently explore a design space in search of better solutions for a large spectrum of optimization problems.

NOMAD is at its best when applied to blackbox functions (see Figure 1.1). Such functions are typically the result of expensive computer simulations which

- have no exploitable property such as derivatives,

- may be contaminated by noise,

- may fail to give a result even for feasible points.

NOMAD is a C++ implementation of the Mesh Adaptive Direct Search (MADS) algorithm [7, 16, 18] designed for constrained optimization of blackbox functions in the form
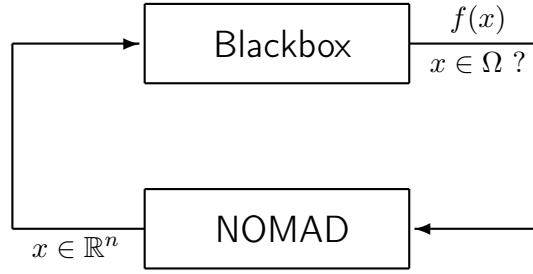
Figure 1.1: NOMAD blackbox optimization.

$$\min_{x \in \Omega} f(x) \tag{1.1}$$

where the feasible set $\Omega = \{x \in X : c_j(x) \leq 0, j \in J\} \subset \mathbb{R}^n$, $f, c_j : X \to \mathbb{R} \cup \{\infty\}$ for all $j \in J = \{1, 2, \ldots, m\}$, and where X is a subset of $\mathbb{R}^n$.

1.2   Basics of the MADS algorithm

At the core of NOMAD resides the Mesh Adaptive Direct Search (MADS) algorithm. As the name implies, this method generates iterates on a series of meshes with varying size. A mesh is a discretization of the space of variables. However, also as the name implies, the algorithm performs an adaptive search on the meshes including controlling the refinement of the meshes. The reader interested in the rather technical details should read [16].

The objective of each iteration of the MADS algorithm, is to generate a trial point on the mesh that improves the current best solution. When an iteration fails to achieve this, the next iteration is initiated on a finer mesh.

Each iteration is composed of two principal steps called the SEARCH and the POLL steps [16]. The SEARCH step is crucial in practice because it is so flexible, but it is a difficulty for the theory for the same reason. SEARCH can return any point on the underlying mesh, but of course, it is trying to identify a point that improves the current best solution.

The POLL step is more rigidly defined, though there is still some flexibility in how this is implemented. The POLL step generates trial mesh points in the vicinity of the best current solution. Since the POLL step is the basis of the convergence analysis, it is the part of the algorithm

where most research has been concentrated.

A high-level presentation of MADS is shown in the pseudo-code below.

Algorithm 1: High-level presentation of MADS

Initialization: Let $x_0 \in \mathbb{R}^n$ be an initial point and set the iteration counter $k \leftarrow 0$
Main loop:
repeat
    SEARCH on the mesh to find a better solution than x_k
    if *the* SEARCH *failed* **then**
        POLL on the mesh to find a better solution than x_k
    if *a better solution than x_k was found by either the* SEARCH *or the* POLL **then**
        call it x_{k+1} and coarsen the mesh
    else
   set $x_{k+1} = x_k$ and refine the mesh
    Update parameters and set $k \leftarrow k + 1$
until *Stopping criteria is satisfied*;

In addition NOMAD includes the following algorithms:

- A MIXED VARIABLE PROGRAMMING (MVP) algorithm to optimize with respect to mixtures of discrete, continuous, and categorical decision variables (see Section 7.1).

- A BiMADS (BI-OBJECTIVE MESH ADAPTIVE DIRECT SEARCH) algorithm to consider a bi-objective version of (1.1) (see Section 7.2).

- A VARIABLE NEIGHBORHOOD SEARCH (VNS) algorithm (see Section 7.6) to escape local minima.

- Three algorithms for parallel executions (see Section 7.4).

1.3   Using NOMAD

NOMAD has no graphical user interface
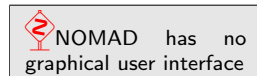
NOMAD does not provide a graphical user interface to define and perform optimization. Minimally, users must accomplish several tasks to solve their own optimization problems:

- Create a custom blackbox program(s) to evaluate the functions f and c_j
  OR embed the functions evaluations in `C++` source code to be linked with the NOMAD library.

- Create the optimization problem definition in a parameter file
  OR embed the problem definition in `C++` source code to be linked with the NOMAD library.

- Launch the execution at the command prompt
  OR from another executable system call.

Users can find several examples provided in the installation package and described in this user guide to perform customization for their problems. The installation procedure is given in Chapter 2. New users should refer to Chapter 3 to get started. The most important instructions to use NOMAD are in Chapter 4. In addition, tricks that may help solving specific problems and improve NOMAD efficiency are presented in Chapter 5. Advanced parameters and functionalities are presented in Chapters 6 and 7.

1.4   Licence

NOMAD is a free software application released under the GNU Lesser General Public License v 3.0. As a free software application you can redistribute and/or modify NOMAD source codes under the terms of the GNU Lesser General Public License.

For more information, please refer to the local copy of the licence obtained during installation. For additional information you can contact us or visit the Free Software Foundation website.

1.5   Contact us

> Contact information:
> École Polytechnique de Montréal - GERAD
> C.P. 6079, Succ. Centre-ville, Montréal (Québec) H3C 3A7 Canada
> e-mail: nomad@gerad.ca
> fax : 1-514-340-5665

All queries can be submitted by email at `nomad@gerad.ca`. In particular, feel free to ask technical support for problem specification (creating parameter files or integration with various types of simulations) and system support (installation and plateform-dependent problems).

Support and
bug report:
`nomad@gerad.ca`

Bug reports and suggestions are valuable to us! We are committed to answer to posted requests as quickly as possible.

1.6 Supported platforms and environments

NOMAD source codes are in `C++` and are identical for all supported platforms.

For convenience, the NOMAD installation packages are customized depending on the platform. The *Mac OS X* and *Windows* installation packages contain executables to quickly start using NOMAD without having to compile the sources. The *Mac OS X* version of the executable is compiled with `Apple LLVM version 5.0` (`clang++`) and is compatible with *Mac OS X* 10.10. The *Windows* version of the executable is compiled with *Visual Studio C++ 2010* but execute on any *Windows* version even if *Visual Studio* is not installed.

The *Linux* installation package contains no executable but the source code includes a standard makefile for compilation. The compilation has been tested with gcc (g++), version 4.

NOMAD supports parallel evaluations of blackboxes. This capability can be obtained by compiling a parallel version of the source code using the message passing interface (*MPI*) or by providing block evaluation of blackboxes. Details on how to proceed are provided in Sections 7.4 and 7.3.

A *MATLAB* version can be obtained from the source code (see Section 2.4.2). In addition, a *MATLAB* version for *Windows* (binaries) can be obtained at OPTI Toolbox website.

> **Tested operating systems and environments:**
>
> - *Unix, Linux & Mac OS X*
>
> - *Windows* XP and *Windows* 7
>
> - *MATLAB 2013a* or above for *Windows* x86 (32bit) and *Windows* x64 (64bit)
>
> The installation procedure is presented in Chapter 2.

1.7 Authors and fundings

The development of NOMAD started in 2001, and was funded in part by AFOSR, CRIAQ, FQRNT, LANL, NSERC, the Boeing Company, and ExxonMobil Upstream Research Company.

Developers of the methods behind NOMAD include

- Mark A. Abramson (abramson@mathematics.byu.edu>), Bringham Young University.

- Charles Audet (www.gerad.ca/Charles.Audet), GERAD and Département de mathématiques et de génie industriel, École Polytechnique de Montréal.

- J.E. Dennis Jr. (www.caam.rice.edu/~dennis), Computational and Applied Mathematics Department, Rice University.

- Sébastien Le Digabel (www.gerad.ca/Sebastien.Le.Digabel), GERAD and Département de mathématiques et de génie industriel, École Polytechnique de Montréal.

- Christophe Tribes, www.gerad.ca and Département de mathématiques et de génie industriel, École Polytechnique de Montréal.

The library for dynamic surrogates (SGTELIB) has been developed by Bastien Talgorn (bastien-talgorn@fastmail.com), McGill University, Montreal. The SGTELIB is included in NOMAD since version 3.8.0.

Version 3.5.1 (and above) of NOMAD is developed by Christophe Tribes. Version 3.0 (and above) was developed by Sébastien Le Digabel. Previous versions were written by Gilles Couture.

1.8   Acknowledgments

The developers of NOMAD wish to thank Florian Chambon, Mohamed Sylla and Quentin Reynaud, all from ISIMA, for their contribution to the project during Summer internships, and to Anthony Guillou and Dominique Orban for their help with AMPL, and their suggestions.

Some features of NOMAD have been developed under the impulsion of enthusiastic users/developers. A special thank to Maud Bay, Eve Bélisle, Vincent Garnier, Michal Kvasnička, Alexander Lutz, Rosa-Maria Torres-Calderon, Yuri Vilmanis, Martin Posch, Etienne Duclos, Emmanuel Bigeon, Walid Zghal, Jerawan Armstrong, Stéphane Alarie and Klaus Truemper for their feedbacks and tests that significantly contributed to improve NOMAD. We also wish to thank Pascal Côté for his contribution in the development of the Python interface *pyNomad* and Jonathan Currie for the development of the foundations for a strong NOMAD interface for *MATLAB*.

Finally, many thanks to the TOMS anonymous referees for their useful comments which helped a lot to improve the code and the text of [44].

1.9   Type conventions

The following conventions are used in this document:

- *Software and operating systems names are typeset in this font.*

- NOMAD is typeset in uppercase.

- `Program codes, program executables, shell commands and environment variables are typeset in this font.`

- `Parameter names are typeset in this font using uppercase.`

- ALGORITHM NAMES ARE TYPESET IN THIS FONT.

- Important information is highlighted in a box like this.

Chapter 2

Software installation and test

The installation procedure depends on the platform you are using. Please refer to the NOMAD website for downloading *Windows*, *Linux / Unix*, or *Mac OS X* versions.

This chapter contains the installation procedures for the supported platforms and describes the content of the installation package. Please refer to the section that fits your needs.

In addition, you can find a *Perl* script in `%NOMAD_HOME%\utils\Run_TestSuite` (*Windows*) or `$NOMAD_HOME/utils/Run_TestSuite` to perform automatic tests once the installation is completed.

2.1   *Windows* installation

To start the installation, double-click on the downloaded file (`NOMAD_setup.exe`), and follow the instructions.

Defining environment variables   allows a more convenient access to NOMAD. *Windows* environment variables are set automatically during installation. The `%NOMAD_HOME%` environment variable contains the path to the installation directory. Also, depending on the options selected during installation, a directory containing examples and a copy of the source codes may have been created along with a `%NOMAD_EXAMPLES%` environment variable that contains the path to

this examples directory.

However, the examples directory and the corresponding environment variable are set only for the current user account during installation. Hence, other users of the computer need to perform two additional operations after installation is completed:

- Copy the %NOMAD_HOME%\examples directory into a convenient location where write permission are granted. This is because the %NOMAD_HOME% may be a read-only directory and running examples requires write permission.

- Set the %NOMAD_EXAMPLES% environment variable to where the examples have been copied. This is achieved through the |Control Panel|System|Advanced|Environment variables| start menu or by searching for 'environment variable'. First, click on the button to create a new environment variable for the current user. Then add the name NOMAD_EXAMPLE and put in the 'variable' field the path where examples have been copied.

> *Windows* installation for additional users requires some extra operations
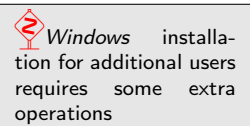
Testing the installation. Depending on the option selected during the installation, this is alternatively done by

> 1 Double clicking on the *NOMAD.3.8.0* icon on the desktop,
>
> 2 Or clicking on the *NOMAD.3.8.0* icon in the *NOMAD.3.8.0* Start Menu,
>
> 3 Or by starting a cmd shell window and typing
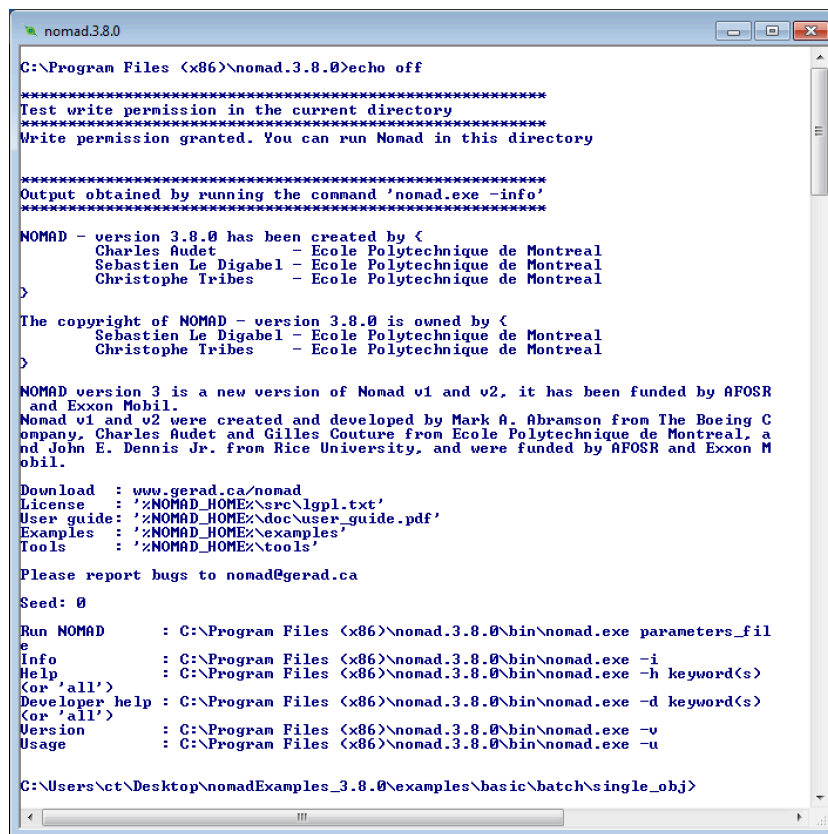>   "%NOMAD_HOME%\bin\nomad.exe" -info
>
> This test displays NOMAD general information as in Figure 2.1.

NOMAD binaries are copied during the installation. Nevertheless, information on how to recompile the source codes is provided in Section 4.3.1.

2.2   *Mac OS X* installation

For *Mac OS X*, open the disk image and copy the NOMAD directory into your Applications folder. We suggest that the user chooses an installation directory with no blank space in the name to ease the creation of environment variables. Also choose directories for which you have the adequate write permissions. Please note that the provided binaries are for OS X v10.10 and may not work on other OS X versions. In that case, you can perform your own compilation of NOMAD (see below).

Defining environment variables allows more convenient access to NOMAD. The first variable to be defined should be $NOMAD_HOME, whose value is the path to the directory where

Figure 2.1: Result of the installation test for *Windows*.

NOMAD has been installed. This variable is used by the makefiles provided in the examples and is assumed to be defined in this document. Another environment variable to set is the `$PATH` variable where `$NOMAD_HOME/bin` should be added. This way, you may just type `nomad` at the command prompt to execute NOMAD.

Here are some examples on how to modify your environment variables according to the shell you are using:

> **For bash shell**, add the following lines in the file `.profile` located in your home directory:
> ```
> export NOMAD_HOME=YOUR_NOMAD_DIRECTORY
> export PATH=$NOMAD_HOME/bin:$PATH
> ```
>
> ---
>
> **For csh or tcsh shell**, add the following lines to the file `.login`:
> ```
> setenv NOMAD_HOME YOUR_NOMAD_DIRECTORY
> setenv $NOMAD_HOME/bin:$PATH
> ```
>
> ---
>
> To activate the variables, at the command prompt, enter the command
> `source .profile` or
> `source .login`, or simply log out and log in.

Unix/Linux/Mac OS X
`$NOMAD_HOME` is **required for compiling examples**

Compilation of source codes is possible if the *gcc* compiler is installed on the machine (if not, install *Xcode* from Apple developer Web site):

> In a terminal window, do `cd $NOMAD_HOME/install` and execute the `./install.sh` command.
>
> ---
>
> This script automatically compiles the code and generates the NOMAD executable in `$NOMAD_HOME/bin` and the NOMAD shared object (so) library in `$NOMAD_HOME/lib`.
>
> ---
>
> The script also detects if *MPI* is installed. If so, the parallel NOMAD executable and library are generated in the same directories as the scalar version.

If your prefer to use another C++ compiler than the one provided in *GNU Compiler Collection (GCC)*, you will need to modify the `makefile` in `$NOMAD_HOME/src`.

Test the installation in a terminal window by entering:

> `nomad -info` at the command prompt. The output of the command should be similar to the one depicted by Figure 2.2

```
> nomad -info


NOMAD - version 3.8.0 has been created by {
Charles Audet       - Ecole Polytechnique de Montreal
Sebastien Le Digabel - Ecole Polytechnique de Montreal
Christophe Tribes    - Ecole Polytechnique de Montreal
}

The copyright of NOMAD - version 3.8.0 is owned by {
Sebastien Le Digabel - Ecole Polytechnique de Montreal
Christophe Tribes    - Ecole Polytechnique de Montreal
}

NOMAD version 3 is a new version of NOMAD v1 and v2, it has been funded by AFOSR and Exxon Mobil.
Nomad v1 and v2 were created and developed by Mark A. Abramson, Charles Audet, Gilles Couture
and John E. Dennis Jr., and were funded by AFOSR and Exxon Mobil.


Download  : www.gerad.ca/nomad
License   : '$NOMAD_HOME/src/lgpl.txt'
User guide: '$NOMAD_HOME/doc/user_guide.pdf'
Examples  : '$NOMAD_HOME/examples'
Tools     : '$NOMAD_HOME/tools'

Please report bugs to nomad@gerad.ca

Seed: 0

Run NOMAD       : $NOMAD_HOME/bin/nomad parameters_file
Info            : $NOMAD_HOME/bin/nomad -i
Help            : $NOMAD_HOME/bin/nomad -h keyword(s) (or 'all')
Developer help  : $NOMAD_HOME/bin/nomad -d keyword(s) (or 'all')
Version         : $NOMAD_HOME/bin/nomad -v
Usage           : $NOMAD_HOME/bin/nomad -u
```

Figure 2.2: Output obtained when testing the installation on *Linux / Unix* and *Mac OS X*.

2.3 *Unix* and *Linux* installation

For *Unix* and *Linux*, decompress the downloaded zip file where you want to install NOMAD.

Please note that NOMAD has been tested with *gcc* compiler. If your prefer to use another compiler, you will need to modify the `makefile` in `$NOMAD_HOME/src`.

Defining environment variables allows more convenient access to NOMAD. The first variable to be defined should be `$NOMAD_HOME`, whose value is the path to the directory where NOMAD has been installed. This variable is used by the makefiles provided in the examples and is assumed to be defined in this document. Another environment variable to set is the `$PATH` variable where `$NOMAD_HOME/bin` should be added. This way, you may just type `nomad` at the command prompt to execute NOMAD. Here are some examples on how to modify your environment variables according to the shell you are using:

> **For bash shell**, add the following lines in the file `.profile` located in your home directory:
> ```
> export NOMAD_HOME=YOUR_NOMAD_DIRECTORY
> export PATH=$NOMAD_HOME/bin:$PATH
> ```
> ------
> **For csh or tcsh shell**, add the following lines to the file `.login`:
> ```
> setenv NOMAD_HOME YOUR_NOMAD_DIRECTORY
> setenv $NOMAD_HOME/bin:$PATH
> ```
> ------
> To activate the variables, at the command prompt, enter the command
> `source .profile` or
> `source .login`, or simply log out and log in.

Unix/Linux/Mac OS X
`$NOMAD_HOME` is
required for compiling examples

Compilation of source codes must be performed to obtain NOMAD binaries (executables and libraries). The shared object libraries are `libnomad.so` and `libsgtelib.so`.

> In a terminal window, do `cd $NOMAD_HOME/install` and execute the `./install.sh` command.
>
> ───
>
> This script automatically compiles the code and generates the NOMAD executable in `$NOMAD_HOME/bin` and the library in `$NOMAD_HOME/lib`.
>
> ───
>
> The script also detects if *MPI* is installed. If so, the parallel NOMAD executable and library are generated in the same directories as the scalar version.

Test the installation by entering:

> `nomad -info` at the command prompt. The output of the command should be similar than the content of Figure 2.2

2.4 *MATLAB* installation

Two *MATLAB* versions of NOMAD can be obtained (*OPTI Toolbox* version and *GERAD* version). Please note that the version available from the OPTI Toolbox website and the GERAD version installed from the source files may be different. Also, the NOMAD command usage are slightly different between the two versions. Please refer to the documentation distributed with the selected version.

2.4.1 *OPTI Toolbox* version

A *MATLAB* version of NOMAD can be downloaded at the OPTI Toolbox website. Please note that the package contains binaries only for *Windows*.

The overall installation including all OPTI provided solvers can be tested by running the test at the command prompt. After installation is completed successfully, NOMAD can be tested alone by typing `nomad('-v')` or `nomad('-info')`.

For additional information concerning installation or utilization please refer to the documentation provided in the OPTI Toolbox package or contact us.

2.4.2   *GERAD version*

It is possible to generate NOMAD binaries for *MATLAB* from NOMAD source files (*Windows*) or NOMAD shared object library (*Mac OS X* and *Linux*) and the `nomadmex.cpp` main file. This procedure may fail due to compatibility issue from *Matlab-MEX* supported and compatible compilers, and the `C++` compiler installed on your machine. Please check this issue before requesting support.[1]

The following procedure must be strictly followed. **In particular, pay attention to the differences when using the *Windows* environment (step 2).**

Start *MATLAB* and enter `mex -setup` at the command prompt.
You must select the Option Template file best suited for the compiler of your choice.

Change the working directory for
`$NOMAD_HOME/examples/interfaces/Matlab_MEX` or
`%NOMAD_EXAMPLES%\examples\interfaces\Matlab_MEX` for *Windows*

Enter the command
`GERAD_NOMAD_build`.

Test the installation with commands: `nomad('-info')` and
`test_nomad_gerad`

The compilation of NOMAD generates a binary file `nomad.mexmaci64` or `nomad.mexw64` depending on the plateform. Please note that the `mex -setup` command is required to generate the options file to control which compiler to use, the compiler and link command options, and the runtime libraries to link against. In some situation the option file may require some minor adjustments to work properly with your installation.

Also, make sure to change the `path` of *MATLAB* to include the

`$NOMAD_HOME/examples/interfaces/Matlab_MEX` or
`%NOMAD_EXAMPLES%\examples\interfaces\Matlab_MEX` (*Windows*) directory. Alternatively, you can move the files `nomad.m`, `nomad.mex***` and `nomadset.m` in the directory of your choice.

---

[1]For example, information for *MATLAB 2012a* and *Linux* is provided at
http://www.mathworks.com/support/compilers/R2012a/glnxa64.html.

Some examples of how to set and run NOMAD are presented in the file `test_nomad_gerad.m`.

2.4.3 Utilization of NOMAD for *MATLAB*

The `nomad` function usage is obtained by typing the command `help nomad`. Please note that parameters are set using a given *MATLAB* function called `nomadset`. Usage of this function is described by typing the command `help nomadset`. Once parameters are set they can be passed as an argument of the `nomad` function. Help on parameters can be obtained by typing the command `nomad('-h PARAM_NAME')`. Parameter names are the same as the standalone NOMAD version.

Two NOMAD functionalities are not available in the present *MATLAB* version: use of categorical variables with changing problem structure (nature and number of variables) and parallel execution using the `MPI` parallel version. Unlike in the previous version (3.6.2 and earlier), the current version partly supports categorical variables. A directory called `test_categorical` contains the same example as in `$NOMAD_HOME/advanced/categorical/batch`. In this example, the structure of the problem (number and nature of variables) cannot be changed when providing neighboring points. Problems with categorical variables that influence the structure of the problem, as the one in `$NOMAD_HOME/advanced/categorical/single_obj`, cannot be solved in the current *MATLAB* version.

2.5 *pyNomad* interface compilation

> The Python inter-face requires Python 2.7 and Cython
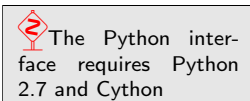
Since version 3.8.0, a Python interface for NOMAD is provided for *Mac OS X* and *Linux*. Some examples and source codes are provided in `$NOMAD_HOME/interfaces/pyNomad_beta`. The compilation procedure requires that NOMAD shared object library is located `$NOMAD_HOME/lib` and relies on Python 2.7 and Cython 0.24 or higher. A simple way to make it work is to first install the Anaconda package.

Please note that not all functionalities of NOMAD are available in PyNomad (beta version). NOMAD parameters are provided in a list of strings using the same syntax as used in the NOMAD parameter files (see examples provided in the dedicated directory).

To build the `PyNomad.so` interface library execute the following command at the prompt in the dedicated directory:
`python setup_PyNomad.py build_ext --inplace`.

To install the library for the current user the command is:
`python setup_PyNomad.py install --user`.

```
>> test_nomad_gerad

-------------------------------------------------------------------
 This is NOMAD v3.8.0
 Authors: C. Audet, S. Le Digabel and C. Tribes
 MEX Interface (GERAD) J. Currie 2012 and C. Tribes 2017

 Problem Properties:
 # Decision Variables:              2
 # Number of Objectives:            1
 # Number of Nonlinear Constraints:    0
-------------------------------------------------------------------

MADS run {

BBE OBJ

1 909.0000000000
8 12.5000000000
17 3.6000000000
31 3.5764000000
32 3.5104000000
33 3.3184000000
35 2.1787890625
44 2.0937971921
45 1.8996640001
50 1.8414478336
51 1.7659289041
60 1.7596628176
61 1.7543346241
67 1.7254458801
69 1.3811794321
72 1.1027884321
81 1.0820160000
82 1.0117237041
83 0.6441350625
92 0.5274037456
93 0.2970466321
98 0.2813428736
99 0.2435006561
104 0.2363232976
117 0.2363232976

} end of run (min mesh size)

blackbox evaluations                     : 117
best feasible solution                   : ( 0.518 0.262 ) h=0 f=0.236323
-------------------------------------------------------------------
>>
```

Figure 2.3: Output obtained when running NOMAD for *MATLAB* on a test case.

Several tests and examples are proposed in the directory to check that everything is up and running.

2.6   Installation directory

Figure 2.4 illustrates the content of the $NOMAD_HOME directory once the installation is completed.
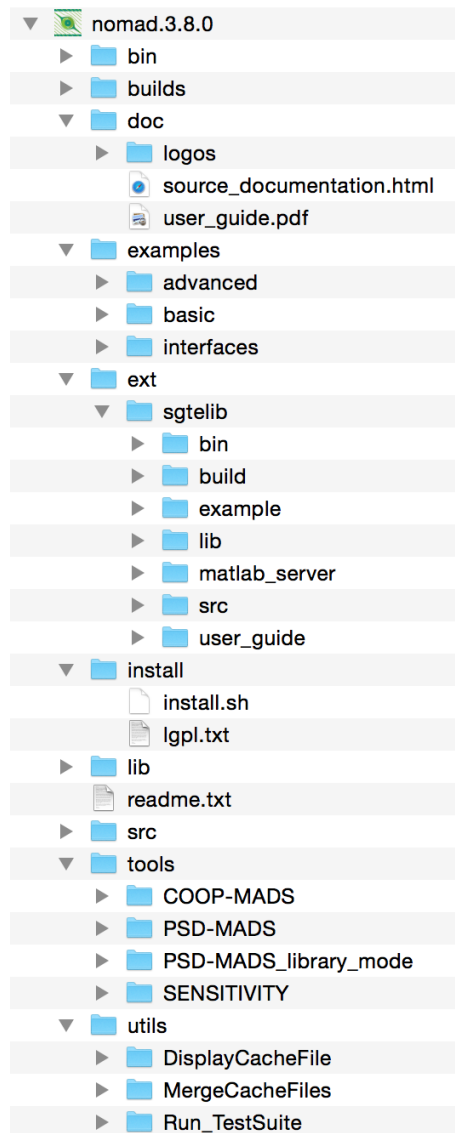
Figure 2.4: Directory structure of the NOMAD package.

Part II

BASIC NOMAD USAGE

Chapter 3

Getting Started

NOMAD is an efficient tool for simulation-based design optimizations provided in the form

$$\min_{x \in \Omega} f(x) \tag{3.1}$$

where the feasible set $\Omega = \{x \in X : c_j(x) \le 0, j \in J\} \subset \mathbb{R}^n$, $f, c_j : X \to \mathbb{R} \cup \{\infty\}$ for all $j \in J = \{1, 2, \ldots, m\}$, and where X is a subset of $\mathbb{R}^n$. The functions f and c_j, $j \in J$, are typically blackbox functions whose evaluations require computer simulation.

NOMAD can be used in two different modes: **batch mode** and **library mode**. The batch mode is intended for a basic usage and is briefly presented below (more details will be provided in Section 4.1), while the library mode allows more flexibility and will be presented in Section 4.3.

This chapter explains how to get started with NOMAD in batch mode. The following topics will be covered:

- How to create a blackbox program.

- How to provide parameters for defining the problem and displaying optimization results.

- How to conduct optimization.

Running the examples provided during the installation requires to have a `C++` compiler installed on your machine.

Basic compilation instructions will be provided for *GCC* (the GNU Compiler Collection) and for *Microsoft Visual Studio*.

When using the *Windows* version, it is assumed that NOMAD examples are in a directory for which the user has write permission and the path is `%NOMAD_EXAMPLES%`. This is obtained during installation with default options or can be set afterwards as described in Section 2.1.

3.1   How to create blackbox programs

To conduct optimization in batch mode the users must define their separate blackbox program coded as a stand-alone program. Blackbox program executions are managed by NOMAD with system calls.

In what follows we use the example in the `$NOMAD_HOME/examples/basic/batch/single_obj` (or `%NOMAD_EXAMPLES%\examples\basic\batch\single_obj` for *Windows*). This example optimization problem has a single objective, 5 variables, 2 nonlinear constraints and 8 bound constraints:

$$\min_{x \in \mathbb{R}^5} f(x) = x_5$$

$$\text{subject to} \quad \begin{cases} c_1(x) = \sum_{i=1}^{5}(x_i - 1)^2 - 25 & \leq 0 \\ c_2(x) = 25 - \sum_{i=1}^{5}(x_i + 1)^2 & \leq 0 \\ \qquad\qquad\qquad x_i & \geq -6 \quad i = 1, 2, \ldots, 5 \\ \qquad\qquad\qquad x_1 & \leq 5 \\ \qquad\qquad\qquad x_2 & \leq 6 \\ \qquad\qquad\qquad x_3 & \leq 7 \;. \end{cases}$$

The blackbox programs may be coded in any language (even scripts) but must respect **NOMAD format**:

1. The blackbox program must be callable in a terminal window at the command prompt and take the input vector file name as a single argument. For the example above, the blackbox executable is `bb.exe`, one can execute it with the command `./bb.exe x.txt` (*Linux/Unix/Mac OS X*) or `bb.exe x.txt` (*Windows*). Here `x.txt` is a text file containing a total of 5 values.

2. NOMAD will manage the creation of the **input file consisting of one value for each variable separated by space** and the execution of the blackbox program.

3. The blackbox program must return the evaluation values by displaying them in the **standard output** (default) or by writing them in an output file (see Section 6.2 about advanced parameters). It must also **return an evaluation status of 0** to indicate that the evaluation went well. Otherwise NOMAD considers that the evaluation has failed.

4. The minimum number of values displayed by the blackbox program corresponds to the number of constraints plus one (or two for bi-objective problems) representing the objective function(s) that one seeks to minimize. The constraints values correspond to left-hand side of constraints of the form $c_j \leq 0$ (for example, the constraint $0 \leq x_1 + x_2 \leq 10$ must be displayed with the two quantities $c_1(x) = -x_1 - x_2$ and $c_2(x) = x_1 + x_2 - 10$).

Blackbox programs must comply with **NOMAD format**

A valid blackbox:
- takes an input vector file as single argument,
- reads space-separated values in input vector file,
- returns evaluation values on standard output or file,
- returns an evaluation status.

The blackbox `C++` program of the previous example to evaluate the objective and the two constraints for a given design vector is given in Figure 3.1.

With *GNU* compiler `gcc`, the blackbox compilation and test are as follows:

1. Change directory to `$NOMAD_HOME/examples/basic/batch/single_obj`.

2. Compile the blackbox program with the following command `g++ -o bb.exe bb.cpp`.

3. Test the executable with the text file `x.txt` containing '0 0 0 0 0' by entering the command `bb.exe x.txt`.

4. This test should display '0 -20 20', which means that the point $x = (0\ 0\ 0\ 0\ 0)^T$ has an objective value of $f(x) = 0$, but is not feasible, since the second constraint is not satisfied ($c_2(x) = 20 > 0$).

```cpp
#include <cmath>
#include <iostream>
#include <fstream>
#include <cstdlib>
using namespace std;

int main ( int argc , char ** argv ) {

  double f = 1e20, c1 = 1e20 , c2 = 1e20;
  double x[5];

  if ( argc >= 2 ) {
    c1 = 0.0 , c2 = 0.0;
    ifstream in ( argv[1] );
    for ( int i = 0 ; i < 5 ; i++ ) {
      in >> x[i];
      c1 += pow ( x[i]-1 , 2 );
      c2 += pow ( x[i]+1 , 2 );
    }
    f = x[4];
    if ( in.fail() )
      f = c1 = c2 = 1e20;
    else {
      c1 = c1 - 25;
      c2 = 25 - c2;
    }
    in.close();
  }
  cout << f << " " << c1 << " " << c2 << endl;
  return 0;
}
```

Figure 3.1: Example of a basic blackbox program. This code corresponds to the file `bb.cpp` in `$NOMAD_HOME/examples/basic/batch/single_obj`.

With *Microsoft Visual C++*, the blackbox compilation and test are as follows:

1. Start the *Microsoft Visual C++* command prompt window (see in `|Start Menu|Microsoft Visual Studio 20xx|`).

2. Change directory to `"%NOMAD_EXAMPLES%\examples\basic\batch\single_obj"`.

3. Compile the blackbox program with the following command `cl.exe bb.cpp /EHsc`.

4. Test the executable with the text file `x.txt` containing '0 0 0 0 0', by entering the command `bb.exe x.txt`.
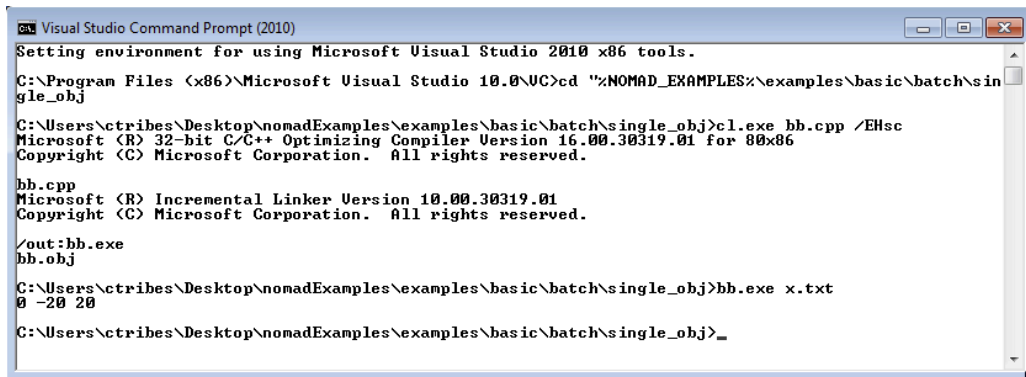
```
> cd $NOMAD_HOME/examples/basic/batch/single_obj
> g++ -o bb.exe bb.cpp
> more x.txt
0 0 0 0 0
> ./bb.exe x.txt
0 -20 20
```

Figure 3.2: Example of a blackbox compilation and execution using GNU Compiler for $NO-MAD_HOME/examples/basic/batch/single_obj.

5. This test should display '0 -20 20', which means that the point $x = (0\ 0\ 0\ 0\ 0)^T$ has an objective value of $f(x) = 0$, but is not feasible, since the second constraint is not verified $(c_2(x) = 20 > 0)$.

Figure 3.3: Example of a blackbox compilation and execution using *Microsoft Visual C++ 2010* Compiler for %NOMAD_EXAMPLES%\examples\basic\batch\single_obj.

The order of the displayed outputs must correspond to the order defined in the parameter file (see Section 3.2). If variables have bound constraints, they must be defined in the parameters file and should not appear in the blackbox code.

3.2   How to provide parameters

In batch mode, the **parameters** are provided in a text file using **predefined keywords** followed by one or more argument. Here are some of the most important parameters defining an optimization problem (without brackets):

- The number of variables (`DIMENSION n`).

- The name of the blackbox executable that outputs the objective and the constraints (`BB_EXE bb_name`).

- Bounds on variables are defined with the `LOWER_BOUND lb` and `UPPER_BOUND ub` parameters.

- The output types of the blackbox executable: objective and constraints (`BB_OUTPUT_TYPE obj cons1...consM`).

- A starting point (`X0 x0`).

- An optional stopping criterion (`MAX_BB_EVAL max_bb_eval`, for example). If no stopping criterion is specified, the algorithm will stop as soon as the mesh size reaches a given tolerance.

- Any entry on a line is ignored after the character '#'.

The order in which the parameters appear in the file or their case is unimportant.

Batch mode parameters are provided in a file as `KEYWORD argument(s)`

Help on parameters is accessible at the command prompt:

`$NOMAD_HOME/bin/nomad -h param_name` (*Linux*/*Mac OS X*/*Unix*).

`"%NOMAD_HOME%\bin\nomad.exe" -h param_name` (*Windows*).

The two constraints defined in the parameters file in Figure 3.4 are of different types. The first constraint $c_1(x) \leq 0$ is treated by the PROGRESSIVE BARRIER approach (PB), which allows constraint violations. The second constraint, $c_2(x) \leq 0$, is treated by the EXTREME BARRIER approach (EB) that forbids violations. Hence, evaluations not satisfying extreme barrier constraints are simply not considered when trying to improve the solution.

In the example above, the algorithmic parameters of NOMAD need not to be set because default values are considered. This will provide the best results in most situations.

```
   DIMENSION      5                # number of variables

   BB_EXE         bb.exe           # 'bb.exe' is a program that
   BB_OUTPUT_TYPE OBJ PB EB        # takes in argument the name of
                                   # a text file containing 5
                                   # values, and that displays 3
                                   # values that correspond to the
                                   # objective function value (OBJ),
                                   # and two constraints values g1
                                   # and g2 with g1 <= 0 and
                                   # g2 <= 0; 'PB' and 'EB'
                                   # correspond to constraints that
                                   # are treated by the Progressive
                                   # and Extreme Barrier approaches
                                   # (all constraint-handling
                                   #  options are described in the
                                   #  detailed parameters list)

   X0             ( 0 0 0 0 0 )    # starting point

   LOWER_BOUND    * -6             # all variables are >= -6
   UPPER_BOUND    ( 5 6 7 - - )    # x_1 <= 5, x_2 <= 6, x_3 <= 7
                                   # x_4 and x_5 have no bounds

   MAX_BB_EVAL    100              # the algorithm terminates when
                                   # 100 blackbox evaluations have
                                   # been made
```

Figure 3.4:   Example of a basic parameters file extracted from $NO-MAD_HOME/examples/basic/batch/single_obj/param.txt. The comments in the file describes some of the syntactic rules to provide parameters.

3.3   How to conduct optimization

Optimization is conducted by starting NOMAD executable in a command window with the parameter file name given as argument. To illustrate the execution, the example provided in $NOMAD_HOME/examples/basic/batch/single_obj/ is considered:

> $NOMAD_HOME/bin/nomad param.txt (*Linux/Mac OS X/Unix*)
>
> "%NOMAD_HOME%\bin\nomad.exe" param.txt (*Windows*)

The outputs are provided in Figures 3.5 and 3.6.

```
> cd $NOMAD_HOME/examples/basic/batch/single_obj
> ls
bb.cpp  bb.exe  param.txt  x.txt
>$NOMAD_HOME/bin/nomad param.txt

NOMAD - version 3.8.0 has been created by {
Charles Audet       - Ecole Polytechnique de Montreal
Sebastien Le Digabel - Ecole Polytechnique de Montreal
Christophe Tribes   - Ecole Polytechnique de Montreal
}

The copyright of NOMAD - version 3.8.0 is owned by {
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}

NOMAD version 3 is a new version of Nomad v1 and v2, it has been funded by AFOSR and Exxon Mobil.
Nomad v1 and v2 were created and developed by Mark A. Abramson, Charles Audet and ...

Download  : www.gerad.ca/nomad
License   : '$NOMAD_HOME/src/lgpl.txt'
User guide: '$NOMAD_HOME/doc/user_guide.pdf'
Examples  : '$NOMAD_HOME/examples'
Tools     : '$NOMAD_HOME/tools'

Please report bugs to nomad@gerad.ca

Seed: 0

MADS run {

BBE ( SOL ) OBJ

  2 ( 0.0000000000 1.0000000000 1.0000000000 -1.0000000000 1.0000000000 ) 144.0000000000 (PhaseOne)
  4 ( 0.0000000000 3.0000000000 2.0000000000 -2.0000000000 1.0000000000 ) 0.0000000000 (PhaseOne)
  4 ( 0.0000000000 3.0000000000 2.0000000000 -2.0000000000 1.0000000000 ) 1.0000000000
 20 ( 2.0000000000 1.0000000000 3.0000000000 -1.0000000000 -3.0000000000 ) -3.0000000000
 57 ( 1.0000000000 1.0000000000 1.0000000000 1.0000000000 -4.0000000000 ) -4.0000000000
100 ( 1.0000000000 1.0000000000 1.0000000000 1.0000000000 -4.0000000000 ) -4.0000000000

} end of run (max number of blackbox evaluations)

blackbox evaluations                    : 100
best infeasible solution (min. violation): ( 0.98 1 1 1.2 -4 ) h=0.0404 f=-4
best feasible solution                   : ( 1 1 1 1 -4 ) h=0 f=-4
>
```
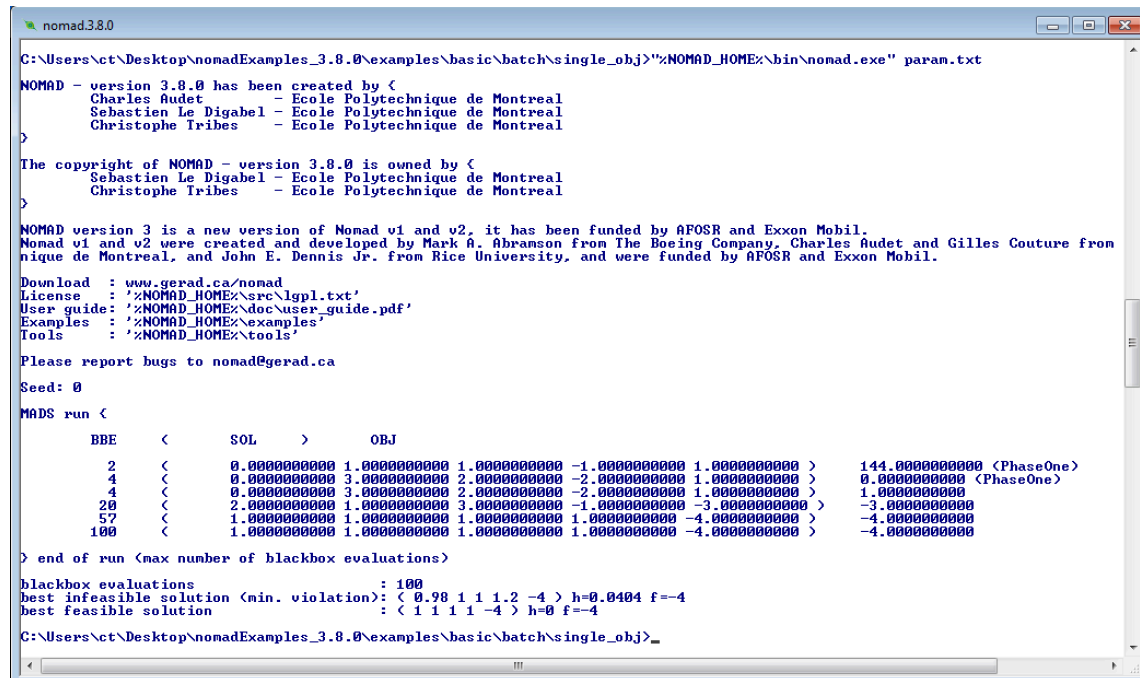
By default only improving evals are displayed

Figure   3.5:   Output   of   NOMAD   execution   on   problem
$NOMAD_HOME/examples/basic/batch/single_obj (*Linux/Mac OS X/Unix*).

By default only improving evals are displayed

Figure 3.6: Output of NOMAD execution on problem %NOMAD_EXAMPLES%\examples\basic\batch\single_obj (*Windows*).

Chapter 4

How to use NOMAD

This chapter describes how to use NOMAD for solving blackbox optimization problems. Functionalities of NOMAD that are considered more advanced such as bi-objective optimization, categorical variables, sensitivity analysis and parallel modes are presented in Chapter 7.

> New users are encouraged to first read the Getting Started chapter to understand the basics of NOMAD utilization.

> Many examples are provided in $NOMAD_HOME/examples with typical optimization outputs.

Batch mode is presented first, followed by a description of the basic parameters to setup and solve the majority of optimization problems that NOMAD can handle. The library mode is described in Section 4.3.

NOMAD should be cited with references [4, 44]. Other relevant papers by the developers are accessible through the NOMAD website www.gerad.ca/nomad.

4.1   Optimization in batch mode

The batch mode allows to separate the evaluation of the objectives and constraints by the blackbox program from NOMAD executable. This mode has the advantage that if your blackbox program crashes, it will not affect NOMAD: The point that caused this crash will simply be tagged as a blackbox failure.

Handling crashes in library mode requires special attention to isolate the part of code that may generate crashes. And, in general, using the library mode will require more computer programming than the batch mode. However, the library mode offers more options and flexibility for blackbox integration and management of optimization (see Section 4.3).

The different steps for solving your problem in batch mode are:

1. Create a directory for your problem. The problem directory is where the NOMAD command is executed. It is a convenient place to put the blackbox executable, the parameters file and the output files, but those locations can be customized.

2. Create your blackbox evaluation, which corresponds to a program (a binary executable or a script). This program can be located in the problem directory or not. This program outputs the objectives and the constraints for a given design vector. If you already have a blackbox program in a certain format, you need to interface it with a wrapper program to match the **NOMAD specifications** (see Section 3.1 for blackbox basics and Section 4.2.1 for more details).

3. Create a parameters file, for example `param.txt`. This file can be located in the problem directory or not (see Section 4.2 for more details).

4. In the problem directory, start the optimization with a command like
   `$NOMAD_HOME/bin/nomad param.txt` (*Linux/Mac OS X/Unix*) or
   `"%NOMAD_HOME%\bin\nomad.exe" param.txt` (*Windows*).

4.2   Basic parameters description

This section describes the basic parameters for the optimization problem definition, the algorithmic parameters and the parameters to manage output information. Additional information can be obtained by executing the command

`$NOMAD_HOME/bin/nomad -h` (*Linux/Mac OS X/Unix*) or
`"%NOMAD_HOME%\bin\nomad.exe" -h` (*Windows*), to see all parameters, or
`$NOMAD_HOME/bin/nomad -h PARAM_NAME` (*Linux/Mac OS X/Unix*) or
`"%NOMAD_HOME%\bin\nomad.exe" -h PARAM_NAME` (*Windows*) for a particular parameter.

The remaining content of a line is ignored after the character '#'. Except for the file names, all strings and parameter names are case insensitive (`DIMENSION 2` is the same as `Dimension 2`). File names refer to files in the problem directory. To indicate a file name containing spaces, use quotes (`"name"` or `'name'`). These names may include directory information relatively to the problem directory. The problem directory will be added to the names, unless the '$' character is used in front of the names. For example, if a blackbox executable is run by the command `python script.py`, define parameter `BB_EXE $python script.py`.

Some parameters consists of a list of variable indices taken from 0 to $n-1$ (where n is the number of variables). Variable indices may be entered individually or as a range with format '`i-j`'. Character '`*`' may be used to replace 0 to $n-1$. Other parameters require arguments of type boolean: these values may be entered with the strings `yes`, `no`, `y`, `n`, `0`, or `1`. Finally, some parameters need vectors as arguments, use (`v1 v2 ...   vn`) for those. The strings '`-`', '`inf`', '`-inf`' or '`+inf`' are accepted to enter undefined real values (NOMAD considers $\pm\infty$ as an undefined value).

Parameters are classified into problem, algorithmic and output parameters, and provided in what follows. Additional information about parameters and algorithms are provided in Subsection 4.2.1. The advanced parameters and special functionalities of NOMAD are presented in Chapters 6 and 7.

Problem parameters

name	arguments	description	default
BB_EXE	list of strings; see 4.2.1	blackbox executables (required in batch mode)	none
BB_INPUT_TYPE	see 4.2.1	blackbox input types	* R (all real)
BB_OUTPUT_TYPE	see 4.2.1	blackbox output types (required)	none
DIMENSION	integer	n the number of variables (required, $n \le 1000$)	none
LOWER_BOUND	see 4.2.1	lower bounds	none
UPPER_BOUND	see 4.2.1	upper bounds	none

Algorithmic parameters

name	arguments	description	default
DIRECTION_TYPE	see 4.2.1	type of directions for the poll	ORTHO
F_TARGET	reals, f or (f1 f2)	NOMAD terminates if $f_i(x_k) \leq$ fi for all objective functions	none
INITIAL_MESH_SIZE	see 4.2.1	δ_0 [16]	none
INITIAL_POLL_SIZE	see 4.2.1	Δ_0 [16]	r0.1 or based on X0
LH_SEARCH	2 integers: p0 and pi	LH (LATIN-HYPERCUBE) SEARCH (p0: initial, pi: iterative); see 4.2.1 (7.2 for bi-objective)	none
MAX_BB_EVAL	integer	maximum number of blackbox evaluations; see 7.2 for bi-objective	none
MAX_TIME	integer	maximum wall-clock time (in seconds)	none
TMP_DIR	string	temporary directory for blackbox i/o files; see 4.2.1	problem directory
X0	see 4.2.1	starting point(s)	best point from a cache file or from an initial LH SEARCH

Output parameters

name	arguments	description	default
CACHE_FILE	string	cache file; if the file does not exist, it will be created	none
DISPLAY_ALL_EVAL	bool	if yes all points are displayed with DISPLAY_STATS and STATS_FILE	no
DISPLAY_DEGREE	integer in $[0, 3]$ or a string with four digits; see 4.2.1	0: no display; 3: full display	1
DISPLAY_STATS	list of strings	what informations is displayed at each success; see 4.2.1	see 4.2.1
HISTORY_FILE	string	file containing all trial points with format (x1 x2 ... xn) on each line; includes multiple evaluations	none
SOLUTION_FILE	string	file to save the current best feasible point or the final best infeasible point if no feasible point has been obtained followed by a warning message	none
STATS_FILE	a string file_name plus a list of strings	the same as DISPLAY_STATS but for a display into file file_name	none

4.2.1   Additional information for some parameters

Parameters `BB_OUTPUT_TYPE` **and** `BB_EXE`

In batch mode, `BB_EXE` indicates the names of the blackbox executables.

A single string may be given if a single blackbox is used and gives several outputs. It is also possible to indicate several blackbox executables.

A blackbox program can return more than one function (`BB_OUTPUT_TYPE`):

```
BB_EXE          bb.exe               # defines that 'bb.exe' is an
BB_OUTPUT_TYPE OBJ EB EB             # executable with 3 outputs
```

The possible arguments for `BB_OUTPUT_TYPE` are described in page .

A mapping between the names of the blackbox programs and the `BB_OUTPUT_TYPE` may be established to identify which function is returned by which blackbox:

```
BB_EXE          bb1.exe bb2.exe      # defines two blackboxes
BB_OUTPUT_TYPE OBJ      EB           # 'bb1.exe' and 'bb2.exe'
                                     # with one output each
```

Blackbox program names can be repeated to establish more complex mapping:

```
BB_EXE    bb1.exe bb2.exe bb2.exe    # defines TWO blackboxes
                                     # NO duplication if names are repeated
BB_OUTPUT_TYPE EB OBJ PB             # bb1.exe  has one output
                                     # bb2.exe  has two outputs
                                     # bb1.exe is executed first.
                                     #!!!  If EB constraint is feasible then
                                     #!!!         bb2.exe is executed.
```

```
                                          #!!!  If EB constraint not feasible then
                                          #!!!       bb2.exe is not launched.
```

A path can precede the blackbox program but spaces are not accepted in the path:

```
  BB_EXE "dir_of_blackbox/bb.exe"
```

To prevent NOMAD from adding a path, the special character '$' should be put in front of a command:

```
  BB_EXE "$python bb.py"           # the blackbox is a python
                                   # script: it is run with
                                   # command
                                   # 'python PROBLEM_DIR/bb.py'
```

```
  BB_EXE "$nice bb.exe"            # to run bb.exe
                                   # in nice mode on X systems
```

Blackbox input parameter `BB_INPUT_TYPE`

This parameter indicates the types of each variable. It may be defined once with a list of n input types with format (t1 t2 ... tn) or several times with index ranges and input types. Input types are values in {R, C, B, I} or {Real, Cat, Bin, Int}. R is for real/continuous variables, C for categorical variable, B for binary variables, and I for integer variables. The default type is R.

For categorical variables (mixed integer variable) please refer to Section 7.1.

Blackbox output parameter `BB_OUTPUT_TYPE`

This parameter characterizes the values supplied by the blackbox, and in particular tells how constraint values are to be treated. The arguments are a list of m types, where m is the number of outputs of the blackbox. At least one of these values must correspond to the objective

function that NOMAD minimizes. If two outputs are tagged as objectives, then the BIMADS algorithm will be executed. Other values typically are constraints of the form $c_j(x) \leq 0$, and the blackbox must display the left-hand side of the constraint with this format.

> A terminology is used to describe the different types of constraints [18]:
>
> > EB constraints correspond to constraints that need to be always satisfied (*unrelaxable constraints*). The technique used to deal with those is the EXTREME BARRIER approach, consisting in simply rejecting the infeasible points.
> >
> > PB, PEB, and F constraints correspond to constraints that need to be satisfied only at the solution, and not necessarily at intermediate points (*relaxable constraints*). More precisely, F constraints are treated with the FILTER approach [15], and PB constraints are treated with the PROGRESSIVE BARRIER approach [18]. PEB constraints are treated first with the PROGRESSIVE BARRIER, and once satisfied, with the EXTREME BARRIER [20].
> >
> > There may be another type of constraints, the *hidden constraints*, but these only appear inside the blackbox during an execution, and thus they cannot be indicated in advance to NOMAD (when such a constraint is violated, the evaluation simply fails and the point is not considered).
>
> If the user is not sure about the nature of its constraints, we suggest using the keyword CSTR, which correspond by default to PB constraints.

There may be other types of outputs. All the types are:

CNT_EVAL	Must be 0 or 1: count or not the blackbox evaluation
EB	Constraint treated with EXTREME BARRIER (infeasible points are ignored).
F	Constraint treated with FILTER approach [15].
NOTHING or –	The output is ignored.
OBJ	Objective value to be minimized.
PB or CSTR	Constraint treated with PROGRESSIVE BARRIER [18].
PEB	Hybrid constraint PB/EB [20].
STAT_AVG	Average of this value will be computed for all blackbox calls (must be unique).
STAT_SUM	Sum of this value will be computed for all blackbox calls (must be unique).

Please note that F constraints are not compatible with CSTR, PB or PEB. However, EB can be combined with F, CSTR, PB or PEB.

Bound parameters `LOWER_BOUND` and `UPPER_BOUND`

Parameters `LOWER_BOUND` and `UPPER_BOUND` are used to define bounds on variables. For example, with $n = 7$,

```
LOWER_BOUND  0-2  -5.0
LOWER_BOUND  3     0.0
LOWER_BOUND  5-6  -4.0
UPPER_BOUND  0-5   8.0
```

is equivalent to

```
LOWER_BOUND ( -5 -5 -5 0 - -4 -4 ) # '-' or '-inf' means that x_4
                                   # has no lower bound
UPPER_BOUND (  8 8 8 8 8 8 inf )   # '-' or 'inf' or '+inf' means
                                   # that x_6 has no upper bound.
```

Each of these two sequences define the following bounds
$$\begin{cases} -5 \leq & x_0 & \leq 8 \\ -5 \leq & x_1 & \leq 8 \\ -5 \leq & x_2 & \leq 8 \\ 0 \leq & x_3 & \leq 8 \\ & x_4 & \leq 8 \\ -4 \leq & x_5 & \leq 8 \\ -4 \leq & x_6 \, . \end{cases}$$

Direction type parameter `DIRECTION_TYPE`

The types of direction correspond to the arguments of parameters `DIRECTION_TYPE`. Up to 4 strings may be employed to describe one direction type.

These 4 strings are s1 in {`ORTHO`,`LT`,`GPS`}, s2 in {∅,`1`,`2`,`N+1`,`2N`}, s3 in {∅,`STATIC`,`RANDOM`, `QUAD`,`NEG`,`UNI`}, and s4 in {∅,`UNIFORM`}. If only 1,2 or 3 strings are given, defaults are considered for the others. Combination of these strings may describe the following 17 direction types:

	s1	s2	s3	s4	direction types
1	ORTHO	1			ORTHOMADS, 1.
2	ORTHO	2			ORTHOMADS, 2.
3	ORTHO				ORTHOMADS, n+1, quad model for (n+1)th dir.
3	ORTHO	N+1			ORTHOMADS, n+1, quad model for (n+1)th dir.
3	ORTHO	N+1	QUAD		ORTHOMADS, n+1, quad model for (n+1)th dir.
4	ORTHO	N+1	NEG		ORTHOMADS, n+1, (n+1)th dir=-sum n first dirs.
5	ORTHO	N+1	UNI		ORTHOMADS, n+1 dirs uniformly distributed
6	ORTHO	2N			ORTHOMADS, 2n.
7	LT	1			LT-MADS, 1.
8	LT	2			LT-MADS, 2.
9	LT	N+1			LT-MADS, n+1.
10	LT				LT-MADS, 2n.
10	LT	2N			LT-MADS, 2n.
11	GPS	BIN			GPS for binary variables.
12	GPS	N+1			GPS, n+1, static.
12	GPS	N+1	STATIC		GPS, n+1, static.
13	GPS	N+1	STATIC	UNIFORM	GPS, n+1, static, uniform angles.
14	GPS	N+1	RAND		GPS, n+1, random.
15	GPS	N+1	RAND	UNIFORM	GPS, n+1, random, uniform angles.
16	GPS				GPS, 2n, static.
16	GPS	2N			GPS, 2n, static.
16	GPS	2N	STATIC		GPS, 2n, static.
17	GPS	2N	RAND		GPS, 2n, random.

GPS directions correspond to the coordinate directions. LT and ORTHO directions correspond to the implementations LT-MADS [16] and ORTHOMADS [7] of MADS. The integer indicated after GPS, LT and ORTHO corresponds to the number of directions that are generated at each poll. The 16 different direction types may be chosen together by specifying DIRECTION_TYPE several times. If nothing indicated, ORTHO is considered for the primary poll, and default direction types for the secondary poll are ORTHO 1 or 2, LT 1 or 2, and GPS N+1 STATIC depending on the value of DIRECTION_TYPE.

Output parameters DISPLAY_DEGREE

Four different levels of display can be set via the parameter DISPLAY_DEGREE, and these levels may be set differently for four different sections of the algorithm (general displays, search and poll displays and displays for each iteration data). The four different levels can be entered with an integer in $[0; 3]$, but also with the strings NO_DISPLAY, MINIMAL_DISPLAY, NORMAL_DISPLAY, or FULL_DISPLAY. If the maximum level of display is set, then the algorithm informations are displayed within indented blocks. These blocks ease the interpretation of the algorithm logs

when read from a text editor.

Output parameters `DISPLAY_STATS` **and** `STATS_FILE`

These parameters display information each time a new feasible incumbent (i.e. a new best solution) is found. `DISPLAY_STATS` displays at the standard output and `STATS_FILE` writes a file. These parameters need a list of strings as argument, **without any quotes**. These strings may include the following keywords:

BBE	Blackbox evaluations.
BBO	Blackbox outputs.
BLK_EVA	Number of blocks of evaluations.
CONS_H	Infeasibility (h).
EVAL	Evaluations (includes cache hits).
MESH_INDEX	Mesh index ℓ [7].
MESH_SIZE	Mesh size parameter δ^k [24] (or Δ_k^m [16]).
OBJ	Objective function value.
POLL_SIZE	Poll size parameter Δ^k [24] (or Δ_k^p [16]).
SGTE	Number of surrogate evaluations.
SIM_BBE	Simulated blackbox evaluations (includes initial cache hits).
SOL	Solution, with format iSOL where i is an optional string: i will be displayed before and after each coordinate. Solution, with format SOLj where j is an optional string: j will be displayed between each coordinate.
STAT_AVG	The AVG statistic (argument STAT_AVG of BB_OUTPUT_TYPE).
STAT_SUM	The SUM statistic defined by argument STAT_SUM for parameter BB_OUTPUT_TYPE.
TIME	Wall-clock time.
VARi	Value of variable i. The index 0 corresponds to the first variable.

In addition, all outputs may be formatted using the `C` style. Possibilities and examples are shown in the following table:

%e	Scientific notation (mantissa/exponent) using e character.
%E	Scientific notation (mantissa/exponent) using E character.
%f	Decimal floating point.
%g	Use the shorter of %e or %f.
%G	Use the shorter of %E or %f.
%d or %i	Integer rounded value.

The number of columns (width) and the precision may also be indicated using also the `C` style as in the following examples:

format	width	precision
%f	auto	auto
%5.4f	5	4
%5f	5	auto
%.4f	auto	4
%.f	auto	0

For example,
`DISPLAY_STATS $BBE$ & ( $SOL, ) & $OBJ$`
displays lines similar to
`$1$ & ( $10.34$ , $5.58$ ) & $-703.4734809$`
which may be copied into LaTeX tables.

The same example with
`DISPLAY_STATS $BBE$ & ( $%5.1fSOL, ) & $%.2EOBJ$`
gives
`$1$ & ( $ 10.3$ , $ 5.6$ ) & $-7.03E+02$`.

In case the user wants to explicitly display the % character, it must be entered using \\%.

Default values are `DISPLAY_STATS BBE OBJ` and `DISPLAY_STATS OBJ` for single and bi-objective optimization, respectively (there is no need to enter `OBJ` twice in order for the two objective values to be displayed).

To write these outputs into the file `output.txt`, simply add the file name as first argument of `STATS_FILE`:
`STATS_FILE output.txt BBE ( SOL ) OBJ`.

Mesh and poll size parameters

The initial poll size parameter Δ_0 is decided by `INITIAL_POLL_SIZE`. In order to achieve the scaling between variables, NOMAD considers the poll size parameter for each variable independently. The initial mesh size parameter δ_0 is decided based on Δ_0. `INITIAL_POLL_SIZE` may be entered with the following formats:

- `INITIAL_POLL_SIZE d0` (same initial mesh size for all variables)

- `INITIAL_POLL_SIZE (d0 d1 ...  d`n`-1)` (for all variables '`-`' may be used, and defaults will be considered)

- `INITIAL_POLL_SIZE i d0` (initial mesh size provided for variable `i` only)

- `INITIAL_POLL_SIZE i-j d0` (initial mesh size provided for variables `i` to `j`)

The same logic and format apply for providing the `INITIAL_MESH_SIZE`, `MIN_MESH_SIZE` and `MIN_POLL_SIZE`.

Note that a more explicit scaling method is available with the advanced parameter `SCALING` (see Section 6.2).

Latin Hypercube search `LH_SEARCH`

When using LATIN HYPERCUBE (LH) search (`LH_SEARCH p_0 p_1` with `p_0` or `p_1` different than zero) for single-objective optimization, `p_0` and `p_1` correspond to the initial number of search points and to the number of search points at each iteration, respectively. For bi-objective optimization this has a slightly different meaning (see Section 7.2)

Temporary directory parameter `TMP_DIR`

If NOMAD is installed on a network file system, with the batch mode use, the cost of read/write files will be high if no local temporary directory is defined. On *Linux/Unix/Mac OS X* systems, the directory `/tmp` is local and we advise the user to define `TMP_DIR /tmp`.

Starting point parameter `X0`

Parameter `X0` indicates the starting point of the algorithm. Several starting points may be proposed by entering this parameter several times. If no starting point is indicated, NOMAD considers the best evaluated point from an existing cache file (parameter `CACHE_FILE`) or from an initial LATIN-HYPERCUBE SEARCH (argument p0 of `LH_SEARCH`).

The `X0` parameter may take several types of arguments:

- A string indicating an existing cache file, containing several points (they can be already evaluated or not). This file may be the same as the one indicated with `CACHE_FILE`. If so, this file will be updated during the program execution, otherwise the file will not be modified.

- A string indicating a text file containing the coordinates of one or several points (values are separated by spaces or line breaks).

- n real values with format (v0 v1 ... vn-1).

- X0 keyword plus integer(s) and one real:

  X0 i v: (i+1)th coordinate set to v.

  X0 i-j v: coordinates i to j set to v.

  X0 * v: all coordinates set to v.

- One integer, another integer (or index range) and one real: the same as above except that the first integer k refers to the (k+1)th starting point.

The following example with $n = 3$ corresponds to the two starting points $(5\ 0\ 0)$ and $(-5\ 1\ 1)$:

```
X0 * 0.0
X0 0 5.0
X0 1 * 1.0
X0 1 0 -5.0
```

4.3 Optimization in library mode

The library mode allows to tailor the evaluation of the objectives and constraints within a specialized executable that contains NOMAD shared object library. For example, it is possible to link your own code with the NOMAD library (provided during installation) in a single executable that can define and run optimization for your problem. Contrary to the batch mode, this has the disadvantage that a crash within the executable (for example during the evaluation of a point) will end the optimization unless a special treatment of exception is provided by the user. But, as a counterpart, it offers more options and flexibility for blackbox integration and optimization management (display, pre- and post-processing, multiple optimizations, user search, etc.).

The library mode requires additional coding and compilation before conducting optimization. First, we will briefly review the compilation of source code to obtain NOMAD binaries (executable and shared object libraries) and how to use library. Then, details on how to interface your own code are presented.

4.3.1 Compilation of the source code

NOMAD source code provided during installation are located in $NOMAD_HOME/src (*Unix/Linux/Mac OS X*) or in %NOMAD_EXAMPLES%\VisualStudio\src (*Windows*). In what follows

it is supposed that you have a write access to the source codes directory. If it is not the case, please consider making a copy in a more convenient location.

For *Unix*, *Linux* and *Mac OS X*, we suggest a compilation procedure using the makefiles provided along with the sources. The makefiles are for *GNU* `gcc` compiler and may need some modifications depending on your system (`C++` compiler and `make` version). Enter the command `make all` from a terminal opened in directory `$NOMAD_HOME/src`. This will create the executable file `nomad` located in `$NOMAD_HOME/bin` and the shared object library file `libnomad.so` in `$NOMAD_HOME/lib`. If the `make` command fails, try `gmake` instead of `make`.

For *Windows*, a console application project for *Microsoft Visual C++ (2010)* (professional or express edition are supposed to be available) is provided for convenience. First, double-click on the `%NOMAD_EXAMPLES%\VisualStudio\nomad.sln` (`Microsoft Visual Studio Solution`). In the menu `Debug` (express edition) on in the menu `Build` (professional) click on `Build Solution`. This will create `nomad.exe` and `nomad.lib` in the `%NOMAD_EXAMPLES%\VisualStudio\bin` and `...\lib` directories.

The Visual Studio projects provided in NOMAD distribution should open without much trouble with versions of Visual Studio following 2010. For further information please refer to this page: [How to: Upgrade Visual C++ Projects to Visual Studio 2015](). Please note that future releases of NOMAD will be upgraded to Visual Studio 2015.

4.3.2   Using NOMAD library

Using the NOMAD routines that are in the pre-compiled NOMAD shared object library (*Unix*/ *Linux*/ *Mac OS X*) or static library (Windows) with a `C++` program requires building an executable. This is illustrated on the example located in the directory
`$NOMAD_HOME/examples/basic/library/single_obj`
or in
`%NOMAD_EXAMPLES%\examples\basic\library\single_obj`.
It is identical to the example shown in Chapter [3](), except that no temporary files are used, and no system calls are made. For this example, just one `C++` source file is used, but there could be a lot more. Other examples can be found in `$NOMAD_HOME/examples` or in `%NO-MAD_EXAMPLES%\examples`.

Building with *Microsoft Visual C++*

The example is provided as the `basic_lib_single_obj` project in the `nomad` solution. First, you must build the `nomad` solution as described before to create NOMAD static library. Then, to build the example, right-click on the `basic_lib_single_obj` project in the solution explorer

Figure 4.1: Outputs obtained for %NOMAD_EXAMPLES%\examples\basic\library\single_obj (*Windows*).

and select build. The resulting executable is located in
%NOMAD_EXAMPLES%\examples\basic\library\single_obj. Execution can be started within *Visual Studio* (professional edition only) or in command shell and will produce the result given in Figure 4.1.

New users of *Microsoft Visual C++* are encouraged to get familiar with the software application first and than create their own project based on the example provided. Please note that important properties can be modified by right-clicking on a project and selecting Properties.

Building with makefile

It is supposed that the environment variable $NOMAD_HOME is defined and NOMAD shared object library is in $NOMAD_HOME/lib. If not, the installation directory of NOMAD must be modified in the makefile. Explanations are given for *GNU* C++ compiler gcc. A basic knowledge of object oriented programming with C++ is assumed.

Let us first try to compile the basic example. In a terminal, change directory to
$NOMAD_HOME/examples/basic/library/single_obj
and type make. The outputs for this examples are given in Figure 4.2

As a first task to create your own executable, a makefile needs to be created for your source code(s). The makefile for the basic example is shown on Figure 4.3. Notice that each line after the symbol ':' has to begin with a tabulation. Such makefiles are given at various places inside the examples directory.

```
> cd $NOMAD_HOME/examples/basic/library/single_obj
> make
   building the scalar version ...
   exe file : basic_lib.exe
> ls
basic_lib.cpp  basic_lib.exe  basic_lib.o  makefile
> ./basic_lib.exe

$ ./basic_lib.exe

MADS run {

BBE ( SOL ) OBJ

  2 ( 0.0000000000 1.0000000000 1.0000000000 -1.0000000000 1.0000000000 ) 144.0000000000 (PhaseOne)
  4 ( 0.0000000000 3.0000000000 2.0000000000 -2.0000000000 1.0000000000 ) 0.0000000000 (PhaseOne)
  4 ( 0.0000000000 3.0000000000 2.0000000000 -2.0000000000 1.0000000000 ) 1.0000000000
 20 ( 2.0000000000 1.0000000000 3.0000000000 -1.0000000000 -3.0000000000 ) -3.0000000000
 57 ( 1.0000000000 1.0000000000 1.0000000000 1.0000000000 -4.0000000000 ) -4.0000000000
300 ( 1.0000000000 1.0000000000 1.0000000000 1.0000000000 -4.0000000000 ) -4.0000000000

} end of run (max number of blackbox evaluations)

blackbox evaluations                    : 300
best infeasible solution (min. violation): ( 0.9999999513 0.9999995812 1.0000005 1.000000065 -4.000000034 )
                                           h=3.381817848e-07 f=-4.000000034
best feasible solution                   : ( 1 1 1 1 -4 ) h=0 f=-4
```

Figure 4.2: Outputs obtained for `$NOMAD_HOME/examples/basic/library/single_obj` (*Linux*).

4.3.3   Definition of the blackbox evaluation

We now describe the other steps required for the creation of the source file (let us call it `basic_lib.cpp`), which includes the header file `nomad.hpp`, and which is divided into two parts: a class for the description of the problem, and the main function. Once compiled with the makefile (type `make` for *Linux*/*Unix*/*Mac OS X*) or with build command in *Visual Studio C++*, the binary file (let us call it `basic_lib.exe`) is created and can be executed.

The use of standard `C++` types for reals and vectors is of course allowed within your code, but it is suggested that you use the NOMAD types as much as possible. For reals, NOMAD uses the class `NOMAD::Double`, and for vectors, the class `NOMAD::Point`. A lot of functionalities have been coded for theses classes, which are visible in files `Double.hpp` and `Point.hpp`. All NOMAD class files are named like the classes and are located in the directory `$NOMAD_HOME/src`. Other NOMAD types (essentially enumeration types) are also defined in `defines.hpp`. Some utility functions on these types can be found in `utils.hpp`. The namespace `NOMAD` is used for all NOMAD types, and you must type `NOMAD::` in front of all types unless you type `using namespace NOMAD;` at the beginning of your program.

Providing the blackbox evaluation of objective and constraints directly in the code avoids the use of temporary files and system calls by the algorithm. This is achieved by defining a derived class (let us call it `My_Evaluator`) that inherits from the class `NOMAD::Evaluator` in single-objective optimization and from `NOMAD::Multi_Obj_Evaluator` in multi-objective mode (see header files `Evaluator.hpp` and `Multi_Obj_Evaluator.hpp`). An example of such a class is shown in Figure 4.5 in section 4.4.

> The blackbox evaluation is programmed in a user-defined class. The objective of this user class is to redefine the virtual method `NOMAD::Evaluator::eval_x()` that will be automatically called by the algorithm.

The prototype of `eval_x()` is given in Figure 4.4. Note that `const` and non-`const` versions of the method are available. The function `eval_x()` should return `true` if the evaluation succeeded, and `false` if the evaluation failed.

The argument `x` (in/out) corresponds to an evaluation point, i.e. a vector containing the coordinates of the point to be evaluated, and also the result of the evaluation. The coordinates are accessed with the operator `[]` (`x[0]` for the first coordinate) and outputs are set with the method `NOMAD::Eval_Point::set_bb_output()` (`x.set_bb_output(0,v)` to set the objective function value to `v` if the objective has been defined at the first position). Constraints must be represented by values c_j for a constraint $c_j \leq 0$. Please refer to files `Eval_Point.hpp` and `Point.hpp` for details about the classes defining NOMAD vectors.

The second argument, the real `h_max` (in), corresponds to the current value of the barrier h_{max} parameter. It is not used in this example but it may be used to interrupt an expensive evaluation if the constraint violation value h grows larger than h_{max}. See [18] for the definition of h and h_{max} and of the PROGRESSIVE BARRIER method for handling constraints. Please refer to Section 6.1 for description of parameters h_{max} and h_{min}.

The third argument, `count_eval` (out), needs to be set to `true` if the evaluation counts as a blackbox evaluation, and `false` otherwise (for example, if the user interrupts an evaluation with the h_{max} criterion before it costs some expensive computations, then set `count_eval` to `false`).

Finally, note that the call to `eval_x()` inside the NOMAD code is inserted into a `try` block. This means that if an error is detected inside the `eval_x()` function, an exception should be thrown. The choice for the type of this exception is left to the user, but `NOMAD::Exception` is available (see `Exception.*pp`). If an exception is thrown by the user-defined function, then the associated evaluation is tagged as a failure and not counted unless the user explicitely set the

flag `count_eval` to true. Additionally, the user-defined function can test on whether `CTRL-C` has been pressed by using the method `NOMAD::Evaluator::get_force_quit()`. This allows managing the termination of a costly black-box evaluation within `eval_x()`.

The virtual method `NOMAD::Evaluator::update_success()` can also be subclassed in the `My_Evaluator` class. The corresponding derived method will be automatically invoked every time a new improvement is made. Note that the automatic calls to this method can be enabled/disabled with `NOMAD::Evaluator_Control::set_call_user_update_success()`.

4.3.4   The main function

Once your problem has been defined, the main function can be written. NOMAD routines may throw C++ exceptions, so it is recommended that you put your code into a `try` block. In addition, functions `NOMAD::begin()` and `NOMAD::end()` must be called at the beginning and at the end of the main function. `NOMAD::Slave::stop_slaves()` also has to be called at the end of the main function if parallelism is used.

Setting parameters

> In library mode, the main function must declare a `NOMAD::Parameters` object. Parameter names are the same as in batch mode but may be defined programmatically. A parameter PNAME is set with the method `NOMAD::Parameters::set_PNAME()`.

In library mode, parameter PNAME is set with `set_PNAME()`.

In order to see all the options attached to a parameter PNAME, use the help
`$NOMAD_HOME/bin/nomad -h PNAME` (*Linux/Unix/Mac OS X*) or
`"%NOMAD_HOME%\bin\nomad.exe" -h PNAME` (*Windows*) or
refer to the list of parameters in Sections 4.2 and 6.1, or to the header file `Parameters.hpp`.

In library mode it is also possible to provide the parameters by reading from a file, with `NOMAD::Parameters::read("param.txt")` where `param.txt` is a valid parameters file. If a directory path is included in the name of the file, this path will be considered as the problem path instead of the default location './'. To display the parameters described by a `NOMAD::Parameters` object p, use the instruction `cout « p « endl;`.

NOMAD types can be used as arguments of `NOMAD::Parameters` functions. An example is given in Figure 4.6. This example is taken from file `basic_lib.cpp` located in `$NOMAD_HOME/examples/basic/library/single_obj` and corresponds to the same parameters as given in Figure 3.4 except for `BB_EXE` which is not required.

> Once that all parameters are set, the method NOMAD::Parameters::check() must be invoked to validate the parameters. The algorithm will not run with a non-checked NOMAD::Parameters object.

If parameters are changed after a first check, check() must be invoked again before a new run can be conducted. Notice that the call to check() may be bypassed by using NOMAD::Parameters::force_check_flag() but only advanced users should use it.

Evaluator declaration and algorithm run

> The MADS algorithm is implemented in the NOMAD::Mads class. Objects of this class are created with a NOMAD::Parameters object and an NOMAD::Evaluator object as arguments.
>
> Once the NOMAD::Mads object is declared, run the algorithm with NOMAD::Mads::run() (or NOMAD::Mads::multi_run() for multi-objective optimization). An example is shown in Figure 4.7.

In the example described in Figure 4.7, the NOMAD::Evaluator object corresponds to an object of type My_Evaluator. A NULL pointer may also be used instead of the NOMAD::Evaluator object: in this case, the default evaluator will be used. Assuming that the parameter BB_EXE has been defined, this default evaluator consists in evaluating the objective function via a separated blackbox program and system calls. When an NOMAD::Evaluator object is used, parameters BB_EXE and SGTE_EXE are ignored. A more advanced NOMAD::Mads constructor with user-created caches is also available in $NOMAD_HOME/src/Mads.hpp.

Access to solution and optimization data

In the example of $NOMAD_HOME/examples/basic/library/single_obj, final information is displayed at the end of NOMAD::Mads::run(). More specialized access to solution and optimization data is allowed.

To access the best feasible and infeasible points, use the methods NOMAD::Mads::get_best_feasible() and NOMAD::Mads::get_best_infeasible(). To access optimization data or statistics, call the method NOMAD::Mads::get_stats() which returns access to a NOMAD::Stats object. Then, use the access methods defined in Stats.hpp. For example, to display the number of blackbox evaluations, write:

```
cout << "bb eval = " << mads.get_stats().get_bb_eval() << endl;
```

4.3.5   Other functionalities of the library mode

Automatic calls to user-defined functions

Virtual methods are automatically invoked by NOMAD at some special events of the algorithm. These methods are left empty by default and you may redefine them so that your own code is automatically called. These virtual methods are defined in the `NOMAD::Evaluator` and `NOMAD::Multi_Obj_Evaluator` classes and are detailed below:

- `NOMAD::Evaluator::list_of_points_preprocessing()`: Called before the evaluation of a list of points (it allows the user to pre-process the points to be evaluated). See `$NOMAD_HOME/src/Evaluator.hpp` for the header of this method.

- `NOMAD::Evaluator::update_iteration()`: Invoked every time a MADS iteration is terminated.

- `NOMAD::Evaluator::update_success()`: Invoked when a new incumbent is found (single-objective) or when a new Pareto point is found (bi-objective).

- `NOMAD::Multi_Obj_Evaluator::update_mads_run()`: For bi-objective problems, this method is called every time a single MADS run is terminated.

It is possible to disable the automatic calls to these methods, with the functions `NOMAD::Mads::enable_user_calls()` and `NOMAD::Mads::disable_user_calls()`, or with the parameters `USER_ CALLS_ENABLED` and `EXTENDED_POLL_ENABLED`. These parameters are automatically set to yes, except during the extended poll for categorical variables and during the VNS search.

Multiple runs

The method `NOMAD::Mads::run()` may be invoked more than once, for multiple runs of the MADS algorithm.

A simple solution for doing that is to declare the `NOMAD::Mads` object, as in Figure 4.8. But, in this case, the cache, containing all points from the first run, will be erased between the runs (since its it created and deleted with `NOMAD::Mads` objects).

Another solution consists in using the `NOMAD::Mads::reset()` method between consecutive runs and to keep the `NOMAD::Mads` object in a more global scope. The method takes two boolean arguments (set to `false` by default), `keep_barriers` and `keep_stats`, indicating if the barriers (true and surrogate) and statistics must be reset between the two runs. An example is shown in Figure 4.9.

> Examples showing multiple MADS runs are provided in the
> `$NOMAD_HOME/examples/advanced/restart` and
> `$NOMAD_HOME/examples/advanced/multi_start` directories. The `multistart` program
> launches multiple instances of MADS with different starting points from a LATIN-HYPERCUBE sampling.

4.4   Interface examples

Blackbox evaluations programs can be in different format. The example directory `$NOMAD_HOME /examples/interfaces` illustrates how to interface NOMAD in the following cases:

- **AMPL**: The interface to the *AMPL* format uses a library developed by Dominique Orban and available at www.netlib.org/ampl/solvers. A `readme.txt` file is given with the example and describes the different steps necessary for the example to work. This example has been written with the help of Dominique Orban and Anthony Guillou.

- **CUTEr**: How to optimize *CUTEr* [39] test problems.

- **DLL**: Blackbox that is coded inside a dynamic library (a *Windows* DLL). Single-objective and bi-objective versions are available.

- **FORTRAN**: Two examples.

  First a blackbox problem coded as a *FORTRAN* routine linked to the NOMAD library.

  Then a more elaborate example mixing *FORTRAN* and the NOMAD library where a *FORTRAN* program is used both to define the problem and to run NOMAD.

- **GAMS**: Optimization on a blackbox that is a *GAMS* [32] program.

- **NOMAD2**: Program to use NOMAD version 3 on a problem originally designed for the version 2. This example has been written by Quentin Reynaud.

- **Matlab**: Please refer to section 2.4.

- **Python**: Please refer to section 2.5.

```
EXE                = basic_lib.exe

COMPILATOR         = g++
COMPILATOR_OPTIONS = -O2 -ansi

LIB_DIR            = $(NOMAD_HOME)/lib
LIB_NOMAD          = libnomad.so

CXXFLAGS           =
ifeq ($(UNAME), Linux)
CXXFLAGS           += -Wl,-rpath,'$(LIB_DIR)'
CXXFLAGS           += -ansi
endif

LDLIBS             = -lm -lnomad
INCLUDE            = -I$(NOMAD_HOME)/src -I$(NOMAD_HOME)/ext/sgtelib/src -I.
COMPILE            = $(COMPILATOR) $(COMPILATOR_OPTIONS) $(INCLUDE) -c
OBJS               = basic_lib.o


ifndef NOMAD_HOME
define ECHO_NOMAD
        @echo Please set NOMAD_HOME environment variable!
        @false
endef
endif


$(EXE): $(OBJS)
        $(ECHO_NOMAD)
        @echo "   building the scalar version ..."
        @echo "   exe file : "$(EXE)
        @$(COMPILATOR) -o $(EXE) $(OBJS) $(LDLIBS) $(CXXFLAGS) -L$(LIB_DIR)
ifeq ($(UNAME), Darwin)
        @install_name_tool -change $(LIB_NOMAD) $(NOMAD_HOME)/lib/ ...
        $(LIB_NOMAD) $(EXE)
endif
```

Figure 4.3: Example of a makefile for a single C++ file linked with the NOMAD library.

```
   bool eval_x ( NOMAD::Eval_Point   & x            ,
                 const NOMAD::Double & h_max       ,
                 bool                 & count_eval   ) const;
```

Figure 4.4: Prototype of method `NOMAD::Evaluator::eval_x()`. A non-const version is also available.

```
class My_Evaluator : public NOMAD::Evaluator {
public:
  My_Evaluator  ( const NOMAD::Parameters & p ) :
    NOMAD::Evaluator ( p ) {}

  ~My_Evaluator ( void ) {}

  bool eval_x ( NOMAD::Eval_Point   & x            ,
                const NOMAD::Double & h_max       ,
                bool                 & count_eval   ) const {
    NOMAD::Double c1 = 0.0 , c2 = 0.0;
    for ( int i = 0 ; i < 5 ; i++ ) {
      c1 += (x[i]-1).pow2();
      c2 += (x[i]+1).pow2();
    }
    x.set_bb_output  ( 0 , x[4]  ); // objective value
    x.set_bb_output  ( 1 , c1-25 ); // constraint 1
    x.set_bb_output  ( 2 , 25-c2 ); // constraint 2

    count_eval = true; // count a blackbox evaluation
    return true;       // the evaluation succeeded
  }
};
```

Figure 4.5: Example of a user class defining a hard-coded blackbox evaluation.

```
// display:
NOMAD::Display out ( std::cout );

// parameters creation:
NOMAD::Parameters p ( out );

p.set_DIMENSION (5);              // number of variables

// definition of output types:
vector<NOMAD::bb_output_type> bbot (3);
bbot[0] = NOMAD::OBJ;
bbot[1] = NOMAD::PB;
bbot[2] = NOMAD::EB;
p.set_BB_OUTPUT_TYPE ( bbot );

// starting point:
p.set_X0 ( NOMAD::Point ( 5 , 0.0 ) );

// lower bounds: all var. >= -6:
p.set_LOWER_BOUND ( NOMAD::Point ( 5 , -6.0 ) );

// upper bounds (x_4 and x_5 have no upper bounds):
NOMAD::Point ub ( 5 );
ub[0] = 5.0;  // x_1 <= 5
ub[1] = 6.0;  // x_2 <= 6
ub[2] = 7.0;  // x_3 <= 7
p.set_UPPER_BOUND ( ub );

p.set_MAX_BB_EVAL (100);     // the algorithm terminates
                             // after 100 bb evaluations

// parameters validation:
p.check();
```

Figure 4.6: Example of parameters creation in library mode.

```
// custom evaluator creation:
My_Evaluator ev ( p );

// algorithm creation and execution:
NOMAD::Mads mads ( p , &ev , cout );
mads.run();
```

Figure 4.7: Evaluator and Mads objects usage.

```
{
  NOMAD::Mads mads ( p , &ev , cout );

  // run #1:
  mads.run();
}

// some changes...

{
  NOMAD::Mads mads ( p , &ev , cout );

  // run #2:
  mads.run();
}
```

Figure 4.8: Two runs of MADS with a `NOMAD::Mads` object at local scope. The cache is erased between the two runs.

```
NOMAD::Mads mads ( p , &ev , cout );
// run #1:
mads.run();

// some changes...
mads.reset();

// run #2:
mads.run();
```

Figure 4.9: Two runs of MADS with a `NOMAD::Mads` object at a more global scope. The cache is kept between the two runs.

Chapter 5

Tricks of the trade

NOMAD has default values for all algorithmic parameters. These values represent a compromise between robustness and performance obtained by developers on sets of problems used for benchmarking. But you might want to improve NOMAD performance for your problem by tuning the parameters or use advanced functionalities. The following sections provide tricks that may work for you.

5.1   Tune NOMAD

Here are a few suggestions for tuning NOMAD when facing different symptoms. The suggestions can be tested one by one or all together.

Symptom	Suggestion	Ref
I want to see more display	Set display degree	page 43
Blackbox manages output file name	Use `BB_REDIRECTION`	see 6.2
Quantifiable constraints	Try PB, EB, PEB or combinations	page 40
Difficult constraint	Try PB instead of EB	4.2.1
	Relax feasibility criterion `H_MIN`	page 68
No initial point	Add a LH search	4.2.1
Variables of widely	Provide scaling	6.2
different magnitudes	Change Δ_0 per variable	page 45
	Tighten bounds	page 42
Many variables	Fix some variables	6.2
	Use $\mathrm{PSD\text{-}MADS}$	7.4
Unsatisfactory solution	Change direction type to $\mathrm{ORTHO\ 2N}$	page 42
	Change initial point	page 46
	Add a VNS search	7.6
	Add a LH search	page 46
	Change direction types	page 42
	Deactivate `SNAP_TO_BOUNDS`	page 70
	Tighten bounds	page 42
	Change Δ_0	page 45
	Modify seeds that affect algorithms	page 72
	Disable models	page 68
	Unable SGTELIB models	page 75
Improvements get negligible	Change stopping criteria	Type `nomad -h stop`
	Disable models	page 68
It takes long to improve f	Decrease Δ_0	page 45
Optimization is time consuming	Perform parallel blackbox evaluations	7.4 and 7.3
	Use surrogate	6.2
	Provide a user search	7.7
Blackbox is not that expensive	Setup maximum wall-clock time	4.2
	Add a VNS search	7.6
	Add a LH search	4.2.1
	Combine direction types	page 42
Bi-objective optimization slow	Treat an objective as a constraint	4.2.1
	Perform parallel blackbox evaluations	7.4
	Set bounds for objectives	4.2.1
Bi-objective optimization	Increase evaluation budget per MADS run	7.2
stops prematurely	Decrease number of MADS run	7.2
	Relax feasibility criterion `H_MIN`	6.1

5.2 Dynamically plot optimization history

Users may want to plot information during NOMAD execution. This can be achieved by implementing the `NOMAD::Evaluator::update_success()` virtual function. You can find an example using *Java* in `$NOMAD_HOME/examples/advanced/plot`.

5.3 Tools to visualize results

What-if scenarios, and sensitivity to constraints can be post analyzed with the tools of Section 7.5.

5.4 Use categorical variables

When variables can be represented by integers, but the numbers do not mean anything and they cannot be logically ordered without further analyses, the variables can be represented using categorical variables. In particular, when your problem has a number of design variables that can vary by selecting a parameter, this parameter can be set as a categorical variable. See Section 7.1.

Part III

ADVANCED NOMAD USAGE

Chapter 6

Advanced parameters

6.1 Parameters description

Advanced parameters are intended to setup optimization problems, algorithmic and output parameters when specific needs are present.

Problem parameters

name	arguments	description	default
`FIXED_VARIABLE`	see 6.2	fixed variables	none
`PERIODIC_VARIABLE`	index range	define variables in the range to be periodic (bounds required)	none
`SGTE_COST`	integer c	the cost of c surrogate evaluations is equivalent to the cost of one blackbox evaluation	∞
`SGTE_EVAL_SORT`	bool	if surrogates are used to sort list of trial points	yes
`SGTE_EXE`	list of strings; see 6.2	surrogate executables	none
`VARIABLE_GROUP`	index range	defines a group of variables; see 6.2	none

Algorithmic parameters

name	arguments	description	default
`ASYNCHRONOUS`	bool	asynchronous strategy for the parallel version; see 7.4	yes
`ANISOTROPIC_MESH`	bool	adapt mesh anisotropy during optimization based on direction of success per variables (ORTHOMADS)	yes
`BB_INPUT_INCLUDE_SEED`	bool	if the random seed is put as the first entry in blackbox input files	no
`BB_INPUT_INCLUDE_TAG`	bool	if the tag of a point is put as an entry in blackbox input files	no
`BB_MAX_BLOCK_SIZE`	integer	maximum size of a block of evaluations; see 7.3	1
`BB_REDIRECTION`	bool	if NOMAD manages the creation of blackbox output files; see 6.2	yes
`CACHE_SEARCH`	bool	enable or disable the cache search (useful with extern caches)	no
`DISABLE`	string	forcefully disables a feature provided as argument; see 6.2	-
`EXTENDED_POLL_ENABLED`	bool	if `no`, the extended poll for categorical variables is disabled	yes
`EXTENDED_POLL_TRIGGER`	real	trigger for categorical variables; value may be relative; see 7.1	`r0.1`
`GRANULARITY`	see 6.2	Granularity of variables	0 (real)
`H_MAX_0`	real	initial value of h_{max} (will be eventually decreased throughout the algorithm)	1E+20
`H_MIN`	real `v`	x is feasible if $h(x) \leq v$	0.0
`H_NORM`	norm type in {`L1`, `L2`, `Linf`}	norm used to compute h	L2
`HAS_SGTE`	bool	indicates if the problem has a surrogate (only necessary in library mode)	no or yes if `SGTE_EXE` is defined
`L_CURVE_TARGET`	real	NOMAD terminates if it detects that the objective may not reach this value	none
`MAX_CACHE_MEMORY`	integer	NOMAD terminates if the cache reaches this memory limit expressed in MB	2000
`MAX_CONSECUTIVE_FAILED_ITERATIONS`	integer	max number of MADS failed iterations	none
`MAX_EVAL`	integer	max number of evaluations (includes cache hits and blackbox evaluations, does not include surrogate eval)	none
`MAX_ITERATIONS`	integer	max number of MADS iterations	none
`MAX_SGTE_EVAL`	integer	max number of surrogate evaluations	none

name	arguments	description	default
MAX_SIM_BB_EVAL	integer	max number of simulated black-box evaluations (includes initial cache hits)	none
MESH_COARSENING_EXPONENT	integer	w^+ [16]	1
MESH_REFINING_EXPONENT	integer	w^- [16]	-1
MESH_TYPE	string in {GMESH, XMESH, SMESH}	The mesh type of MADS (see 6.2)	GMESH
MESH_UPDATE_BASIS	real	τ [16] used for SMESH mesh type	4.0
MIN_MESH_SIZE	see pp. 46	δ_{min} [24] (or Δ^m_{min} [16])	none
MIN_POLL_SIZE	see pp. 46	Δ_{min} [24] (or Δ^p_{min} [16])	none or 1 for int/bin variables
MODEL_EVAL_SORT	bool or string	enable or not the ordering of trial points based on a quadratic model or on models provided by the surrogate library see 6.2	yes
MODEL_SEARCH	bool or string	enable or not the search strategy using quadratic models or models provided by the surrogate library 6.2	yes
MODEL_SEARCH_OPTIMISTIC	bool	if model search is optimistic or not	yes
MULTI_F_BOUNDS	4 reals	see 7.2	none
MULTI_NB_MADS_RUNS	integer	number of MADS runs	see 7.2
MULTI_OVERALL_BB_EVAL	integer	max number of blackbox evaluations for all MADS runs	see 7.2
NEIGHBORS_EXE	string	neighborhood executable for categorical variables in batch mode	none
OPPORTUNISTIC_CACHE_SEARCH	bool	opportunistic strategy for cache search	no
OPPORTUNISTIC_EVAL	bool	opportunistic strategy; see 6.2	yes
OPPORTUNISTIC_LH	bool	opportunistic strategy for LH search; see 7.2 for bi-objective	see 6.2
OPPORTUNISTIC_MIN_EVAL	integer	see 6.2	none
POLL_UPDATE_BASIS	real	β used by xmesh	2.0
RHO	real	ρ parameter of the PROGRESSIVE BARRIER	0.1
SCALING	see 6.2	scaling on the variables	none
SEED	integer in [0,INT_MAX] U {-1} or DIFF	random seed; DIFF or {-1} to define a seed that will be different at each run (PID used)	0
SGTELIB_MODEL_DIVERSIFICATION	positive real	coefficient of the exploration term in the surrogate library problem see 6.2	0.01
SGTELIB_MODEL_TRIALS	positive integer	max number of sgtelib model trials for each search see 6.2	1
SGTELIB_MODEL_DEFINITION	SGTELIB keywords	definition of the surrogate library model see 6.2	see 6.2
SGTELIB_MODEL_DISPLAY	string	Control the display of the sgtelib model search see 6.2	empty string = no display

name	arguments	description	default
SNAP_TO_BOUNDS	bool	snap to boundary trial points that are generated outside bounds	yes
SPECULATIVE_SEARCH	bool	MADS speculative search [16]	yes
STAT_SUM_TARGET	real	NOMAD terminates if STAT_SUM reaches this value	none
STOP_IF_FEASIBLE	bool	NOMAD terminates if it generates a feasible solution	no
USER_CALLS_ENABLED	bool	if no, the automatic calls to user functions are disabled	yes
VNS_SEARCH	bool or real	VNS search; see 7.6	no
MESH_TYPE	{gmesh, xmesh smesh }	The type of mesh; see 6.2	gmesh

Ouptut parameters

name	arguments	description	default
ADD_SEED_TO_FILE_NAMES	bool	if the seed is added to the file names corresponding to parameters HISTORY_FILE, SOLUTION_FILE and STATS_FILE	yes
CACHE_SAVE_PERIOD	integer i	the cache files are saved every i iterations (disabled for bi-objective)	25
CLOSED_BRACE	string	displayed at the end of indented blocks	'}'
DISPLAY_DEGREE	string with four digits, each in $[0;2]$	1st digit: general display; 2nd digit: search display; 3rd digit: poll display; 4th digit: iterative display; example: DISPLAY_DEGREE 0010	1111
INF_STR	string	used to display infinity	'inf'
OPEN_BRACE	string	displayed at the beginning of indented blocks	'{'
POINT_DISPLAY_LIMIT	integer	maximum number of point coordinates that will be displayed at screen (-1 for no limit)	20
SGTE_CACHE_FILE	string	surrogate cache file (cannot be the same as CACHE_FILE)	none
UNDEF_STR	string	used to display undefined values	'-'

6.2   Detailed information for some parameters

Detailed information for some of the parameters are provided in what follows.

Blackbox redirection parameter `BB_REDIRECTION`

If this parameter is set to `yes` (default), NOMAD manages the creation of the blackbox output file when the blackbox is executed via a system call (the redirection '`>`' is added to the system command). If no, then the blackbox must manage the creation of its output file named `TMP_DIR/nomad.SEED.TAG.output`. Values of `SEED` and `TAG` can be obtained in the blackbox input files created by NOMAD and given as first argument of the blackbox, only if parameters `BB_INPUT_INCLUDE_SEED` and `BB_INPUT_INCLUDE_TAG` are both set to yes. Alternatively, the output file name can be obtained from the input file name by replacing the extension '`input`' by '`output`'.
In addition, `TMP_DIR` can be specified by the user. The default `TMP_DIR` is the problem directory.

Parameter `DISABLE`

The `DISABLE` parameter is used to forcefully disable a feature. Two arguments are supported: `MODELS` and `EVAL_SORT`.

`DISABLE MODELS` is equivalent to set: `MODEL_EVAL_SORT no`, `MODEL_SEARCH no` and `DIRECTION_TYPE ORTHO N+1 NEG` (if direction type is set to `ORTHO N+1 QUAD`, which is the default). Please note that this parameter has no default and that extra settings of `MODEL_EVAL_SORT`, `MODEL_SEARCH` and `DIRECTION_TYPE ORTHO N+1 QUAD` will be ignored.

`DISABLE EVAL_SORT` allows ordering of points for evaluation by lexicographic order only. The option disables ordering by model evaluation (`MODEL_EVAL_SORT no`), surrogate evaluation (`SURROGATE_EVAL_SORT no`), success direction, point tag number, user priority, etc. This option has an effect only if the opportunistic strategy is enabled.

Fixed variables parameter `FIXED_VARIABLE`

This parameter is used to fix some variables to a value. This value is optional if at least one starting point is defined. The parameter may be entered with several types of arguments:

- A string indicating a text file containing n values. Variables will be fixed to the values that are not defined with the character '`-`'.

- A vector of n values with format (`v0 v1 ... vn-1`). Again, character '`-`' may be used for free variables.

- An index range if at least one starting point has been defined (see 4.2.1 for practical examples of index ranges).

- An index range and a real value, with format `FIXED_VARIABLE i-j v`: variables `i` to `j` will be fixed to the value `v` (`i-j` may be replaced by `i`).

Parameter `SEED`

Please note that the parameter `HALTON_SEED` present in previous versions is deprecated.

The directions that NOMAD explores during the poll phase are dependent upon the seed. The seed is used to generate a pseudo-random direction on a unit n-dimensional sphere. The user can change the sequence of directions by setting `SEED` to a selected value.

Other aspects of NOMAD may depend on a pseudo-random sequence of numbers depending on selected options: LH SEARCH, GPS and LT directions, evaluation order priority, BiMADS and categorical variables.

Opportunistic strategies `OPPORTUNISTIC_EVAL`, `OPPORTUNISTIC_CACHE_SEARCH` **and** `OPPORTUNISTIC_LH`

The opportunistic strategy consists in terminating the evaluations of a list of trial points at a given step of the algorithm as soon as an improved value is found. This strategy is decided with the parameter `OPPORTUNISTIC_EVAL` and applies to both the poll and search steps. For the LH and Cache searches, the strategy may be chosen independently with `OPPORTUNISTIC_LH` and `OPPORTUNISTIC_CACHE_SEARCH`. If these parameters are not defined, the parameter OP-PORTUNISTIC_EVAL applies to the LH and Cache searches. Other defaults are considered for bi-objective optimization (see 7.2).

When evaluations are performed by blocks (`EVAL_LIST_MAX_BLOCK_SIZE` greater than one) the opportunistic strategy applies after evaluating a block of trial points.

Scaling parameter `SCALING`

Scaling in NOMAD is automatically achieved via the mesh and poll size parameters which are vectors with one value per variable. However, this method relies on the existence of bounds. For the case when no bounds are available, or simply to give the user more control on the scaling, the parameter `SCALING` has been introduced in the version 3.4.

The parameter takes variable indices and values as arguments. During the algorithm, variables are multiplied by their associated value (that is scaled) before an evaluation and the call to `NOMAD::Evaluator::eval_x()`. Outside of this method the variables are unscaled.

All NOMAD outputs (including files) display unscaled values. All variable-related parameters (bounds, starting points, fixed variables) must be specified as unscaled. In a parameters file, the scaling is entered similarly to bounds or fixed variables. It is possible to specify a scaling for some
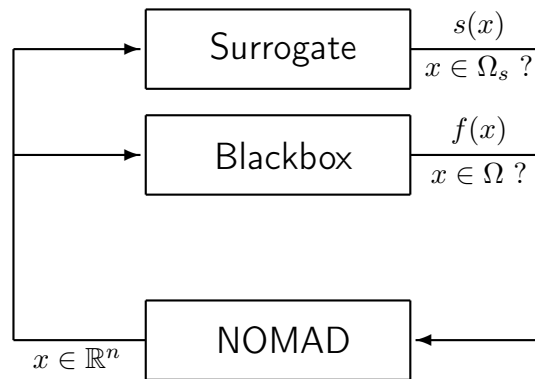
Figure 6.1: Blackbox optimization using surrogates.

variables and none for others. Enter the command $NOMAD_HOME/bin/nomad -h scaling for more details about the use of SCALING.

Executable parameters SGTE_EXE

Static surrogates, or *static surrogate functions*, are cheaper blackbox functions that are used, at least partially, to drive the optimization (see Figure 6.1).

The current version of NOMAD can use static surrogates provided which are not updated during the algorithm and which are provided by the user. See [31] for a survey on surrogate optimization. In addition, a library of dynamic surrogates is also provided. These surrogate are constructed from the evaluations available in the cache and are used for the SEARCH and for sorting points before evaluation (see 6.2)

> Static surrogates are provided by the user

> Dynamic surrogates are included in the surrogate library

In batch mode, the parameter SGTE_EXE associates static surrogate executables with blackbox executables. It may be entered with two formats:

- SGTE_EXE bb_exe sgte_exe to associate executables bb_exe and sgte_exe,

- SGTE_EXE sgte_exe when only one blackbox executable is used. Surrogates must display the same number of outputs as their associated blackboxes.

In the library mode, if a surrogate function is to be used, then its evaluation routine should be coded in the method eval_x() (see Section 4.3.3). First, to indicate that a surrogate can be

computed, the user must set the parameter `HAS_SGTE` to yes, via the method `NOMAD::Para-meters::set_HAS_SGTE()`. Then, in `eval_x()`, the test '`if (x.get_eval_type()==SGTE)`' must be made to differentiate an evaluation with the true function f or with the surrogate.

Group of variables parameter `VARIABLE_GROUP`

By default NOMAD creates one group that combines all continuous, integer, and binary variables, and one group for categorical variables (see Section 7.1).

In batch mode, the `VARIABLE_GROUP` parameter followed by variable indices is used to explicitly form a group of variables. Each group of variable generates its own polling directions. The parameter may be entered several times to define more than one group of variables. Variables in a group may be of different types (except for categorical variables). If a group contains only binary variables, directions of type `NOMAD::GPS_BINARY` will be automatically used.

When using the NOMAD library mode, the groups of variables are created with the method `NO-MAD::Parameters::set_VARIABLE_GROUP()` which has two different prototypes. The method must be called each time a new group is created. For both versions of the function, the set of indices of the variables composing each group is provided as argument of the function. The most complete prototype of `set_VARIABLE_GROUP()` allows to choose the types of these directions, for the primary and secondary polls. The detailed types of directions can be found in file `de-fines.hpp` and the enum type `direction_type`. The simplified prototype uses ORTHOMADS types of directions by default.
Finally the function `NOMAD::Parameters::reset_variable_groups()` may be called to reset the groups of variables. Remember also that after a modification to a `Parameters` object is made, the method `NOMAD::Parameters::check()` needs to be called.

Use of models: `MODEL_SEARCH` **and** `MODEL_EVAL_SORT`

The SEARCH phase of the MADS algorithm can use models of the objectives and constraints that are constructed dynamically from all the evaluations made. The models are used to propose new points to be evaluated with the blackbox. To enable the use of quadratic models, the parameter `MODEL_SEARCH` can be set to yes or `quadratic`. Models from the surrogate library (SGTELIB) can be used by setting `MODEL_SEARCH` to SGTELIB. For additional parameters to control the surrogate library models refer to subsection below and its user guide `$NOMAD_HOME/ext/sgtelib/user_guide/sgtelib/user_guide.pdf`.

Models can also be used to order the points before evaluation with the blackbox. The parameter `MODEL_EVAL_SORT` has the same arguments as the `MODEL_SEARCH` parameter.

Parameters of the SGTELIB

The models provided by the surrogate library are controlled by a series of parameters. The definition of the surrogate model is controlled with the parameter `SGTELIB_MODEL_DEFINITION`. A series of keywords allows to define the type, degree and other specification. Please refer to the SGTELIB user guide
`$NOMAD_HOME/ext/sgtelib/user_guide/sgtelib_user_guide.pdf` for details.

When using the surrogate library models in the SEARCH phase of the MADS algorithm, the coefficient of exploration of the surrogate model search can be specified with the `SGTELIB_MODEL_DIVERSIFICATION` parameter. No exploration is obtained by setting it to 0 and a strong exploration is obtained by setting it to 1, the default value being 0.01. This parameter allows to control the diversification of the points returned by the surrogate model search. In addition, the number of trial points returned by the surrogate problem to be evaluated by the blackbox is controlled by the `SGTELIB_MODEL_TRIALS` parameters. The default value is 1 but more points can be returned. The display of the surrogate library model search is controlled by the `SGTELIB_MODEL_DISPLAY`. The general information on the SGTELIB model search is obtained by setting it to "S", the default being no display. More options are described in the SGTELIB specific user guide. Please note that these parameters have no effect if the `MODEL_SEARCH` is not set to SGTELIB.

Type of mesh parameter `MESH_TYPE`

The MADS algorithm relies on a discretization of the variables space, called the mesh, defined as

$$M^k := \left\{ x + \mathrm{diag}(\delta^k)z : x \in V^k, z \in \mathbb{Z}^n \right\} \tag{6.1}$$

where V^k is the set of all trial points at which the blackbox was evaluated by the start of iteration k, and where $\delta^k = (\delta_1^k, \delta_2^k, \ldots, \delta_n^k)$ is the mesh size vector. The mesh type depends on the definition of the mesh size δ and its update when having evaluation success or failure. Three mesh types are available: GMESH, XMESH and SMESH, the default being GMESH. The older type of mesh is the SMESH which does not support mesh anisotropy (`ANISOTROPIC_MESH`) and specified mesh granularity (see `GRANULARITY` below). The XMESH supports mesh anisotropy but the mesh granularity can not be defined.

Please note that this option has no effect if the `DIRECTION_TYPE` is not set to ORTHO 2N or ORTHO N+1 (default).

Granularity of variables parameter `GRANULARITY`

The `MADS` algorithm handles granular variables, i.e. variables with a controlled number of decimals, when the mesh type is set to `GMESH` (see above). For real numbers the granularity is 0. When this parameter is set to a value greater than 0, the mesh type will be set to `GMESH`. For integers the granularity is automatically set to one.

Chapter 7

Advanced functionalities

7.1 Categorical variables

Categorical variables are discrete variables that can take a finite number of values. These are not integer or binary variables as there is no ordering property amongst the different values that can take the variables. A problem combining categorical variables with continuous variables or even ordinary discrete variables such as integer or binary is called a mixed variables optimization problem.

Examples on categorical variables for a simple portfolio selection problem are provided in `$NOMAD_HOME/examples/advanced/categorical`. A single-objective and a bi-objective version are given in library and batch mode.

The algorithm used by NOMAD to handle mixed variables problems is defined in references [1, 3, 6, 13, 43] and works as follows.

Algorithm

At the end of an iteration where categorical variables are kept fixed, if no improvement has been made, a special step occurs, the *extended poll*. The extended poll first calls the user-provided procedure defining the neighborhood of categorical variables. The procedure returns a list of

points that are neighbors of the current best point (incumbent) such that categorical variables are changed and the other variables may or may not be changed. These points are called the *extended poll points* and their dimension may be different than the current best point, for example when a categorical variable indicates the number of continuous variables.

The functions defining the problem are then evaluated at each of the extended poll points and the objective values are compared to the current best value. If the difference between the objective value at the current iterate and at an extended poll point is less than a parameter called the *extended poll trigger*, this extended poll point is called an *extended poll center* and a new MADS run is performed from this point. This run is called an *extend poll descent* and occurs on meshes that cannot be reduced more than the mesh size at the beginning of the extended poll. If the opportunistic strategy is active, then the different extended poll descents are stopped as soon as a new success is achieved.

If surrogates are available, they can be used to evaluate the neighbors during the extended poll descent. The true functions will then be evaluated only on the most promising points. With surrogates, the extended poll costs at most the same number of true evaluations as the number of neighbors determined by the user-provided procedure.

Mixed variables optimization with NOMAD

We suggest the reader to follow this section along with the reading of the three examples located in `examples/advanced/categorical` that illustrate practical optimizations on mixed variables optimization problems.

In NOMAD, a categorical variable is identified by setting a `BB_INPUT_TYPE` parameter to the value '`C`'. In addition, solving problems with categorical variables requires to define the neighbors of the current best point. In batch mode, this is done by a separate executable (parameter `NEIGHBORS_EXE`) but with the limitation that the number of variables be the same as for the current iterate. See the provided example in `examples/advanced/categorical/batch` for such a case. The limitation of a fixed number of design variables is not present in library mode but requires user programming which is detailed in the remaining of this section.

Programming the method to define the categorical variables neighborhoods relies on a virtual method `NOMAD::Extended_Poll::construct_extended_points()` provided in NOMAD; the user must design its own `NOMAD::Extended_Poll` subclass in which `construct_extended_points()` is coded. This method takes as argument a point (the current iterate) and registers a list of extended poll points (the neighbors of the current iterate) by calling the method `NOMAD::Extended_Poll::add_extended_poll_point()`. In its `main` function, the user gives its own `NOMAD::Extended_Poll` object to the `NOMAD::Mads` object used to

optimize the problem. If no `NOMAD::Extended_Poll` is provided to the `NOMAD::Mads` object, the program will generate an error.

In addition, each point in the algorithm possesses a signature (implemented in the `NOMAD::Signature` class), indicating the characteristics related to the variables: their number, their types, their bounds, their scaling, identification of fixed and periodic variables, and some information on the initial mesh size parameter for each variable. Hence, in the user-provided `NOMAD::Extended_Poll` subclass, for each extended poll point, a signature must be provided. If the extended poll point has the same characteristics than the current best point, the signature of the current best can be used. However, if the number of variables varies according to the value taken by a categorical variable, a new signature must be created and the user is responsible for dealing with the associated memory allocations and deallocations. See the `NOMAD::Signature` class and the example located in `examples/advanced/categorical/single_obj/` for details about creating signatures.

Although the dimension of the problem may change during optimization, the starting points must all have the same characteristics (in particular number and types of variables). For these starting points, the `NOMAD::Parameters` class will automatically create a standard signature. However, if categorical variables are present, the user must explicitly provide starting points. The reason is that the standard poll requires at least one starting point and an initial Latin-Hypercube search cannot be executed to find a starting point (see Section 4.2.1) because it has no reference signature for defining a value for each categorical variable.

Changing the values of the categorical variables is done exclusively during the extended poll phase by providing the neighbors of the current best point. The logic for providing the neighbors is entirely left to the user. For this reason, it is not necessary to provide bounds for the categorical variables whether in the initial description of the problem or when providing extended poll point signatures. A warning message is displayed when the user provides bounds for categorical variables.

The main parameter for mixed variable optimization is the extended poll trigger. Its value is indicated with the parameter `EXTENDED_POLL_TRIGGER`, and may be given as a relative value. The extended poll trigger is used to compare the objective values at an extended poll point y and at the current best point x_k. If $f(y) < f(x_k)+$trigger, then y becomes an extended poll center from which a MADS run is performed. The default trigger value is r0.2, meaning that an extended poll point will become an extended poll center if $f(y)$ is less than $f(x_k) + f(x_k) \times 0.2$. See the function `NOMAD::Extended_Poll::check_trigger()` for the details of this test and for the cases where infeasible points or surrogate evaluations are considered.

Finally, please note that the boolean parameter `EXTENDED_POLL_ENABLED` can simply enable

or disable the extended poll. When disabled, the categorical variables are simply fixed to their initial value.

7.2   Bi-objective optimization

> NOMAD can solve bi-objective optimization problem in search of a Pareto front. Examples of bi-objective problems solved by NOMAD in library and batch mode are given in `$NOMAD_HOME/basic/(batch|library)/bi_obj`.

NOMAD performs bi-objective optimization through the $\textsc{BiMADS}$ algorithm described in [26]. The $\textsc{BiMADS}$ algorithm solves bi-objective problems of the form

$$\min_{x\in\Omega} \qquad F(x) = \big(f_1(x), f_2(x)\big). \tag{7.1}$$

The algorithm launches successive runs of $\textsc{MADS}$ on single-objective reformulations of the problem. An approximation of the Pareto front, or the list of points that are dominant following the definition of [26], is constructed with the evaluations performed during these $\textsc{MADS}$ runs.

Two considerations must be taken into account when generating Pareto fronts: the quality of approximation of the dominant points and the repartition of these points. The quality of approximation may be measured with the `surf` criterion that gives the ratio of the area under the graph of the front relatively to a box enclosing all points (small values indicate a good front).

The quality of the coverage of the Pareto front is measured by the δ criterion, which corresponds to the largest distance between two successive Pareto points.

To define that a problem has two objectives, two arguments of the parameter `BB_OUTPUT_TYPE` must be set to `OBJ`. Then, NOMAD will automatically run the $\textsc{BiMADS}$ algorithm. Additional parameters are:

- `MULTI_F_BOUNDS f1_min f1_max f2_min f2_max` (real values): these 4 values are necessary to compute the `surf` criterion. If not entered or if not valid (for example if `f1_min` is too big), then `surf` is not computed.

- `MULTI_NB_MADS_RUNS` (integer): the number of single-objective $\textsc{MADS}$ runs.

- `MULTI_OVERALL_BB_EVAL` (integer): the maximum number of blackbox evaluations over all $\textsc{MADS}$ runs.

Default values are considered if these parameters are not entered. All other MADS parameters are considered and apply to single MADS runs, with some adaptations:

- The `MAX_BB_EVAL` parameter corresponds to the maximum number of blackbox evaluations for one MADS run.

- The `F_TARGET` parameter is adapted to bi-objective: it must be given with the two values z_1 and z_2. If a point x is generated such that $f_1(x) \leq z_1$ and $f_2(x) \leq z_2$, then the algorithm terminates. In this case, the criterion defines an utopian point. If it can be achieved then the pareto front is a single point.

- The $\mathrm{LATIN\text{-}HYPERCUBE}$ (LH) search (`LH_SEARCH p_0 p_1`): in single-objective optimization, `p_0` and `p_1` correspond to the initial number of search points and to the number of search points at each iteration, respectively. In the bi-objective context, `p_0` is the number of initial search points generated in the first MADS run, and `p_1` is the number of points for the second MADS run. If no LH search is defined by the user, and if only `MULTI_OVERALL_BB_EVAL` is defined, then a default LH search is performed. Moreover, this default LH search is non-opportunistic (`OPPORTUNISTIC_LH` set to no).

- The parameter `SOLUTION_FILE` is disabled.

The NOMAD solution represents an approximation of the Pareto front and is accessible via the `DISPLAY_STATS` or `STATS_FILE` parameters. If `DISPLAY_DEGREE` is greater than 1, then the two measures `surf` and δ are displayed.

For a given budget of blackbox evaluations (`MULTI_OVERALL_BB_EVAL`), if the quality of approximation is desired (small value for `surf`), then single MADS optimizations must terminate after more severe criteria (for example a large number of blackbox evaluations, via `MAX_BB_EVAL`). If a better repartition of the points is desired (small value for δ), then the number of MADS runs should be larger, with less severe stopping criteria on single-objective optimizations.

7.3   Blackbox evaluation of a block of trial points

At different phases of the MADS algorithm, lists of trial points with different sizes are created. For example, having selected the direction type as `ORTHO 2N`, the maximum size of a list during the POLL step will be 2N+2. This list can be partitioned into blocks of trial points to be submitted sequentially for evaluation to a blackbox program. The maximum size of a block of evaluations is controlled by the `BB_MAX_BLOCK_SIZE`. By default, a block contains a single trial point. This can be changed by the user but the blackbox program must support the evaluation of a varying number of trial points, up to `BB_MAX_BLOCK_SIZE`.

Due to the strategy of by-block evaluation, the maximum number of evaluations requested to NOMAD may be exceeded if `BB_MAX_BLOCK_SIZE > 1`. The reason for this behaviour is that block results are analyzed only after completion and the maximum number of evaluations may be exceeded when checking this termination criterion.

The opportunistic strategies (enabled by default) may apply after each block of trial points.

Evaluation of block of trial points can be performed in parallel by the blackbox program. This strategy of parallelization must be setup by the user within the blackbox. Examples are provided in what follows.

7.3.1   Batch mode

In batch mode, NOMAD creates input files which can contain at most `BB_MAX_BLOCK_SIZE` trial points separated by a linebreak. Each point is given as a row of values. The user must provide a blackbox program that can read the input file, evaluate them and output the objective and constraints functions (in the order provided by the `BB_OUTPUT_TYPE` parameter) for each trial point in the same order as provided in the input file (see Fig. 7.1).

A blackbox program may fail to evaluate some of the trial points. When `BB_MAX_BLOCK_SIZE=1`, an empty line in the output file or a line that cannot be interpreted by NOMAD corresponds to a failed evaluation. However, when a block of trial points is submitted the content of the output file must specify which points have failed by using the keyword `FAIL` at the corresponding position in the output file. The keyword `FAIL` should be put only once per trial point independently of the number of outputs given by `BB_OUTPUT_TYPE`. If one value provided in the output file cannot be read by NOMAD then the corresponding trial point is also considered as having failed. The trial points that have failed will not be evaluated again.

A blackbox program can stop prematurely the evaluation of a block of trial points, for example when a best incumbent trial point has been identified within the blackbox. However, to prevent that the remaining trial points of the block be considered as having failed, it is required to explicitly reject them by putting the keyword `REJECT` instead of their corresponding objective and constraint functions. Contrary to trial points that have failed, the rejected ones could be resubmitted later on.

An example of blackbox program written in `Perl` scripting language is provided in the example directory (see Fig. 7.1). This script calls up to 4 instances of the executable `bb.exe` to evaluate 4 trial points in parallel.

```
> cd $NOMAD_HOME/examples/basic/batch/single_obj_parallel
> more x.txt
1 2 3 4 5
0 0 0 0 0
2 2 2 2 2
5 4 3 2 1
> perl parallel_BBWrapper.pl x.txt
5 5 -65
 0 -20 20
 2 -20 -20
 1 5 -65
```

Figure 7.1: Example of a blackbox program evaluating a block of 4 trial points in $NO-
MAD_HOME/examples/basic/batch/single_obj_parallel.

The parameter file that specifies this blackbox program with blocks of 4 trial points is given in
Fig. 7.2.

```
DIMENSION       5               # number of variables

BB_EXE          "$perl parallel_BBWrapper.pl"
BB_MAX_BLOCK_SIZE 4

BB_OUTPUT_TYPE OBJ PB EB

X0              ( 0 0 0 0 0 )  # starting point

LOWER_BOUND     * -6.0           # all variables are >= -6
UPPER_BOUND     ( 5 6 7 - - )  # x_1 <= 5, x_2 <= 6, x_3 <= 7
                                # x_4 and x_5 have no bounds

MAX_BB_EVAL     100             # the algorithm terminates when
                                # 100 black-box evaluations have
                                # been made

DISPLAY_DEGREE 2
```

Figure   7.2:   Example   of   parameter   file   with   BB_MAX_BLOCK_SIZE   in
$NOMAD_HOME/examples/basic/batch/single_obj_parallel.

7.3.2   Library mode

Please refer to `$NOMAD_HOME/examples/basic/library/single_obj_parallel` for an example on how to manage a block of evaluations in parallel using *pThreads* and *Semaphore*.

7.4   NOMAD parallel version

A parallel version of NOMAD can be obtained to perform several blackbox evaluations simultaneously. The parallel version does not support blackbox evaluations for blocks of trial points (see previous section).

7.4.1   Compilation

The NOMAD parallel version is based on the message passing interface (*MPI* [51]). In particular, the *MPI* implementations *openMPI*, *LAM*, *MPICH* and the *Microsoft HPC pack* have been tested. To obtain the parallel binaries (executable and library), NOMAD must link with *MPI*.

For *Linux*, *Unix* or *Mac OS X*, the parallel binaries can be obtained by typing `make mpi` in the `$NOMAD_HOME/src` directory, after ensuring that the command `mpic++` works. The compilation will produce the executable `nomad.MPI` and the shared object library `libnomad.MPI.so`. It is also possible to install all NOMAD binaries (all combinations of scalar/parallel and executables/static libraries) by typing `./install.sh` in the `$NOMAD_HOME/install` directory.

For *Windows*, the parallel binaries can be obtained by compiling NOMAD with *Microsoft Visual C++*. First, you must install a *MPI* implementation (*MPICH* or the *Microsoft HPC pack*, for example). Additional *Microsoft Visual Studio* projects are provided in the `%NOMAD_EXAMPLES%\VisualStudio` directory (`nomad.MPI` and `nomad_lib.MPI`). These projects rely on `MSMPI_INC` and `MSMPI_LIB32` environment variables that are created during the installation of the windows distribution of *MPI*. The settings of these projects may require some modifications if the environment variables for *MPI* are not properly set.

7.4.2   Algorithms

Three algorithms using the parallel version have been developed, namely P-MADS, COOP-MADS, and PSD-MADS. While P-MADS is directly implemented into NOMAD, the two others are programs linked with the NOMAD library (scalar), and are located in the `tools` directory. The parallel version is developed with *MPI* [51] under a master/slaves paradigm.

When creating blackbox problems it is important to keep in mind that the blackboxes will

be called in parallel. So it is crucial that intermediary files possess different names: unique identifiers must be used. For that purpose, in library mode, in your custom `eval_x()` function, use the unique tag of the trial points with the method `NOMAD::Eval_Point::get_tag()`. It is also possible to use `NOMAD::get_pid()` to generate a unique identifier. In batch mode, NOMAD may communicate the seed and the tag of a point to the blackbox executable with the parameters `BB_INPUT_INCLUDE_SEED` and `BB_INPUT_INCLUDE_TAG` (see Section 6.2).

The user must be aware of the random aspect induced by the parallel versions. Even if deterministic directions such as ORTHOMADS are used, two parallel runs may not have the same outputs. Tests have suggested that P-MADS will give similar results as the scalar version, but much faster. The results may sometime be of lower quality due to the fact that the usually efficient opportunistic strategy is not exploited as well as in the scalar version. However, the more evolved COOP-MADS strategy seems to give better results than the scalar version, and faster. The efficiency of the PSD-MADS algorithm is more noticeable on large problems (more than 20 and up to $\simeq$500 variables) on which the other versions are not efficient.

A short description of the methods is given in the following sections, and for a more complete description as well as for numerical results, please consult [45].

For the sake of simplicity, the remaining of the discussion focuses on utilizing the parallel version in the *Linux/Unix/Mac OS X* environments. The same principles apply in the *Windows* environment but the tasks can be performed via the *Microsoft Visual C++* menus and in the command window. Please contact NOMAD support if more details are needed.

The p-MADS method

P-MADS is the basic parallel version of the MADS algorithm where each list of trial points is simply evaluated in parallel.

There are two versions of this method: first the *synchronous* version where an iteration is over only when all evaluations in progress are finished. With this strategy, some processes may be idle. The other version is the *asynchronous* method which consists in interrupting the iteration as soon a new success is made. If there are some evaluations in progress, these are not terminated. If these evaluations lead to successes after they terminate, then the algorithm will consider them and go back to these 'old' points. This version allows no process to be idle. The synchronous and asynchronous versions may be chosen via the parameter `ASYNCHRONOUS` whose default is yes.

The P-MADS executable is named `nomad.MPI` (*Unix / Linux/ Mac OS X*) and is located in

the `bin` directory. It can be executed with the `mpirun` or `mpiexec` commands with the following format under `Linux`:

```
mpirun -np p $NOMAD_HOME/bin/nomad.MPI.exe param.txt
```

where `p` is the number of processes and `param.txt` is a parameters file with the same format as for the scalar version. If you have a number c of processors, then it is suggested to choose `np` to be equal to $c + 1$ (one master and c slaves). It may also be argued that `np` be proportional to the number of polling directions. For example, for a problem with $n = 3$ variables and $2n$ polling directions, each poll is going to generate 6 trial points, and on a 8-processors machine, choosing np=7 may be a better choice than np=9.

The Coop-MADS method

The idea behind the Coop-MADS method is to run several MADS instances in parallel with different seeds so that they all have different behavior.

A special process, called the *cache server*, replaces the usual master process. It implements a parallel version of the cache allowing each process to query if the evaluation at a given point has already been performed. This forbids any double evaluation. The cache server also allows the processes to perform the *cache search*, a special search consisting in retrieving, at each MADS iteration, the currently best known point.

The program given in the `tools` directory implements a simple version of the method where only one type of directions is used with different seeds: LT-MADS or OrthoMADS, with a different random seed.

This program is not precompiled and the user must compile it as any other code using the NOMAD shared object library. Makefiles working for *Linux*, *Unix* and *Mac OS X* are provided. Usage of the program is as follows:

```
mpirun -np p $NOMAD_HOME/tools/COOP-MADS/coopmads param.txt
```

as for P-MADS. Since the cache server is not demanding on computational time, the user can choose np to be the number of available processors plus one.

The PSD-MADS method

> The PSD-MADS method implements a parallel space decomposition of MADS and is is described in [19]. The method aims at solving larger problems than the scalar version of NOMAD.
>
> NOMAD is in general efficient for problems with up to $\simeq$ 20 variables, PSD-MADS has solved problems with up to 500 variables.

In PSD-MADS, each slave process has the responsibility for a small number of variables on which a MADS algorithm is performed. These subproblems are decided by the master process. In the program given in the NOMAD package, as in the original paper, these groups of variables are chosen randomly, without any specific strategy. Concerning other aspects, the program given here is a simplified version of the one used for the SIOPT article [19]. A cache server is also used as in Coop-MADS to forbid double evaluations. A special slave, called the *pollster*, works on all the variables, but with a reduced number of directions. The pollster ensures the convergence of the algorithm.

For *Linux*, *Unix* or *Mac OS X*,   PSD-MADS must be compiled exactly as Coop-MADS, with the available makefile, and it executes with the command:

```
mpirun -np p $NOMAD_HOME/tools/PSD-MADS/psdmads param.txt bbe ns
```

For *Windows*, a *Microsoft Visual Studio* project called psdmads is provided in the %NO-MAD_EXAMPLES%\VisualStudio directory for convenience. This project can be added into the nomad solution in *Microsoft Visual Studio*. Once added, the project can be built to create the psdmads.exe executable in the %NOMAD_EXAMPLES%\examples\PSD-MADS directory. The project relies on MSMPI_INC and MSMPI_LIB32 environment variables that are created during the installation of the windows distribution of *MPI*. The settings of these projects may require some modifications if the environment variables for *MPI* are not properly set. For applying the PSD-MADS method on the example problems provided in %NOMAD_EXAMPLES%\examples \PSD-MADS you have first to open a command window. In this window you can change the directory to %NOMAD_EXAMPLES%\examples\PSD-MADS\G2_10 for example and create the blackbox executable bb.exe from bb.cpp. After that, execute the following command:

```
"%MSMPI_BIN%\mpiexec.exe" -np p "..\..\psdmads.exe" param.txt bbe ns
```

For *Windows*, *Linux* and *Mac OS X*, `bbe` is the maximal number of evaluations performed by each slave and `ns` is the number of variables considered by the slaves. So far, tests suggested that small values for these two parameters lead to good performance. In [19] and [45], `bbe=10` and `ns=2` are considered. The suggested strategy for `np` consists in setting it to the number of processors plus two (master and cache server are not demanding CPU ressources).

Future research will include the design of evolved strategies in order to choose smart groups of variables on which slaves focus.

7.5   Sensitivity analysis

> Sensitivity analysis can perform '**What If**' studies in engineering problems context.
>
> Two tools are available in the NOMAD package to perform sensitivity analyses for constraints, which is a useful tool to grasp more knowledge and see which constraints are important and which may be relaxed or tighten.
>
> Details on the sensitivity analysis with blackboxes and some theoretical results on a smooth case may be consulted in [**?**].

Two tools are available in directory `$NOMAD_HOME/tools/SENSITIVITY` as program sources and can be compiled with makefiles. The tools generate the data necessary to plot objective versus constraint graphs.

The first program is called `cache_inspect` and performs the *simple analysis* which consists in inspecting the cache produced after the execution of NOMAD on a constrained problem (the `CACHE_FILE` parameter must be set). The necessary inputs of this tool are a cache file and two blackbox output indices: one for the objective function, and one for the studied constraint. This last index may refer to a lower or an upper bound: in that case a file containing the bound values must be indicated. The program displays three columns with the values of the studied constraint $c_j(x)$ and of the objective $f(x)$, and a 0/1 flag indicating whether or not the couple $(c_j(x), f(x))$ is non-dominated in the sense of the dominance notion of [26]. An optional parameter allows to display only non-dominated points. These values may be plotted

for example with a *MATLAB* script (one is available in the `cache_inspect` directory).

The second program, called `detailed_analysis`, performs the *detailed analysis*. With this tool, the original problem with constraint $c_j(x) \leq 0$ is replaced with the bi-objective problem

$$\min_{x \in \Omega_j} \quad (c_j(x), \ f(x))$$

$$\text{subjected to:} \quad \underline{c}_j \leq c_j(x) \leq \overline{c}_j$$

where Ω_j is the feasible set Ω minus the constraint. The use of the BiMADS algorithm allows to focus explicitly on the studied constraint in order to obtain a more precise sensitivity. The program takes as inputs a parameters file, the constraint and objective indices, and a cache file. The latter may be empty or not at the beginning of the execution, and it will be updated with the new evaluations. The updated cache file is in fact the output of the program and it may be inspected with the `cache_inspect` tool in order to get the data for the sensitivity graphs. The $\underline{c}_j$ and $\overline{c}_j$ values used to bound the value of $c_j(x)$ may also be specified as input to the tool, as well as a maximum number of evaluations that bypasses the one inside the parameters file. Both programs may be executed without any input which results in the display of the required inputs description.

The typical way of using these tools is as follows: after a single run of MADS, the user uses the simple analysis in order to get a fast preview of the sensitivity without additional blackbox evaluation. After that it is possible to get a more precise analysis on one or several constraints of interest using the detailed analysis, to the cost of additional evaluations.

7.6   Variable Neighborhood Search (VNS)

> The VARIABLE NEIGHBORHOOD SEARCH (VNS) is a strategy to escape local minima.
>
> The VNS search strategy is described in [10]. It is based on the Variable Neighborhood Search metaheuristic [49, 40].

VNS should only be used for problems with several such local optima. It will cost some additional evaluations, since each search performs another MADS run from a perturbed starting point. Though, it will be a lot cheaper if a surrogate is provided via parameter `HAS_SGTE` or `SGTE_EXE`. We advise the user not to use VNS with bi-objective optimization, as the BiMADS algorithm already performs multiple MADS runs.

In NOMAD the VNS search strategy is not activated by default. In order to use the VNS search, the user has to define the parameter `VNS_SEARCH`, with a boolean or a real. This expected

real value is the *VNS trigger*, which corresponds to the maximum desired ratio of VNS blackbox evaluations over the total number of blackbox evaluations. For example, a value of 0.75 means that NOMAD will try to perform a maximum of 75% blackbox evaluations within the VNS search. If a boolean is given as value to `VNS_SEARCH`, then a default of 0.75 is taken for the VNS trigger.

From a technical point of view, VNS is coded as a `NOMAD::Search` sub-class, and it is a good example of how a user-search may be implemented. See files `$NOMAD_HOME/src/VNS_Search.*pp` for details.

7.7 User search

> The default search strategy in NOMAD is based on quadratic models. The surrogate library SGTELIB offers other options for the search. In addition, users may code their own search strategy.

The search must be programmed in a user-defined class. The objective of this user class is to redefine the virtual method `NOMAD::Search::search()` that will be automatically called by the algorithm. The prototype of `search()` is given in Figure 7.3.

```
    void search
    ( NOMAD::Mads            & mads          ,
      int                    & nb_search_pts ,
      bool                   & stop          ,
      NOMAD::stop_type       & stop_reason   ,
      NOMAD::success_type    & success       ,
      bool                   & count_search  ,
      const NOMAD::Eval_Point *& new_feas_inc   ,
      const NOMAD::Eval_Point *& new_infeas_inc  ) ;
```

Figure 7.3: Prototype of method `NOMAD::Search::search()`.

Users can take the example in `$NOMAD_HOME/examples/advanced/user_search` to setup their own search. This example corresponds to a search described in [22]. Other examples on how to design a search strategy can be found in files `$NOMAD_HOME/src/Speculative_Search.*pp`, `LH_Search.*pp`, and `VNS_Search.*pp`. Please note that the MADS theory assumes that trial search points must be lying on the current mesh. Functions `NOMAD::Point::project_to_mesh()`

and `NOMAD::Double::project_to_mesh()` are available to perform such projections.

Part IV

ADDITIONAL INFORMATION

Appendix A

Release notes

A.1 Version 3.8.0

A.1.1 Major changes

- Include the surrogate library to perform the SEARCH phase and sort the evaluation points before calling the blackbox.

- Add the algorithm RobustMads [21] (developper only) for smoothing a noisy objective function of an unconstrained problem using previously evaluated function evaluations.

- Add a mesh type to handle granular variables (GMESH). Allows to select different mesh types: GMESH, XMESH or SMESH.

- Add a *Python* interface for NOMAD.

A.1.2 Minor changes

- Fix bugs.

- Change the stats display for VNS search.

- Add the display of infeasibility (h).

- Add functionnalities and fix bugs in the *MATLAB* interface.

A.2   Version 3.7.3

A.2.1   Minor changes

- Change the text for the copyright.

- NOMAD functionalities are implemented in a shared object library for linux/unix/osx and static library for windows.

- Update the Matlab-mex compilation procedure.

- Allow to provide an extra-parameter passed to the blackbox when using NOMAD in *MAT-LAB*.

- Fix a bug with binary variables.

- Add an intensification mode for polling (specify the number of polling points).

- Change a default setting for quadratic model that could reduce performance.

- Correct some display problem during VNS search.

- Remove TGP model functionalities.

- Fix some issues in relation with categorical variables.

- Modification of the stopping criterion when only integer variables are considered. Allows more local exploration once the mesh size is 1.

- Fix a bug in a rounding function that would affect large numbers.

A.3   Version 3.7.2

A.3.1   Minor changes

- Fix a bug, that affected the software performance, especially for a large number of variables.

- Fix a misleading exception thrown when ending an infeasible bi-objective optimization problem.

- Display a message on exceptions for blackbox evaluations.

- Fix a display problem for execution time.

A.4   Version 3.7.1

A.4.1   Major changes

- Use of a dynamic scaling of the mesh size per variable based on the direction of success during optimization (XMesh) [24].

- ORTHOMADS directions are obtained by a pseudo-random number generator on a unit n-sphere. Halton directions are deprecated. A single seed controls all random aspects of NOMAD.

- Provide partial functionality for categorical variables in the *MATLAB* version.

A.4.2   Minor changes

- The parameter `INITIAL_POLL_SIZE` is added (supersedes `INITIAL_MESH_SIZE`).

- Fix bug when using groups of variables.

- Fix bug when using ORTHOMADS N+1 with fixed variables.

- Fix bug when using evaluations by block.

- Add an example of PSDMADS in library mode.

- Add examples for the *MATLAB* version.

- Fix bug in the *MATLAB* version when using bi-objective.

A.5   Previous versions

Versions 3.6.0 to 3.6.2

- The ORTHOMADS algorithm has been extented to use `N+1` directions in addition of the existing `2N` version.

- Quadratic models are available for BIMADS.

- The *MATLAB* version is distributed as part of NOMAD (version 3.6.2).

- The user guide has been reformatted.

- The installation procedure for *Windows* has been modified to allow copy of examples in a user-specified directory.

- Trial points can be evaluated by block (version 3.6.2).

Version 3.5

- **Quadratic models** are used to improve the algorithm efficiency. Details and benchmarks are available in [33]. A new model search strategy has been implemented in which a local quadratic model is built and optimized in order to provide up to 4 new trial points at each iteration. Also, with model ordering a local quadratic model is built and the points are sorted accordingly to this model so that the most promising points are evaluated first.

- The new parameter `MAX_CONSECUTIVE_FAILED_ITERATIONS` allows to stop the algorithm after a number of unsuccessful iterations of the MADS algorithm.

- When no bounds are present, the initial mesh size (parameter `INITIAL_MESH_SIZE`) has a new default value: instead of being 1 it is now based on the coordinates of the starting point.

- The new parameter `NEIGHBORS_EXE` allows the handling of categorical variables in batch mode. See Section 7.1 and the example located in `examples/advanced/categorical/batch`.

- A series of parameters influencing the behaviour of model search have been renamed for consistency.

- When CTRL-C is pressed an evaluation can be interrupted in library mode within the user provided function `eval_x()`.

- A random number generator have been implemented to allow repeatability of the results on different plateforms.

- A bug in the display format of the stats present when compiling with *Microsoft Visual Studio C++* has been corrected (hexadecimal display).

- A bug when using categorical variables with varying problem dimensionality has been fixed.

- A bug in the values of integers for fine meshes has been fixed.

- A bug in the display stats for the phase one search has been corrected.

Version 3.4

- **Parallelism**: Three parallel algorithms are now available. See Section 7.4 for details.

- All NOMAD types and classes are now included in the namespace `NOMAD`. Consequently enumeration types and constants have their names changed from `_X_` to `NOMAD::X`.

- A documentation has been constructed in the HTML format with the doxygen documentation generator. It is available from the NOMAD website at www.gerad.ca/nomad/doxygen/html.

- NOMAD is now distributed under the *GNU Lesser General Public License (LGPL)*. The license can be found as a text file in the `src` directory or at www.gnu.org/licenses.

- A new parameter `SCALING` allowing the scaling of the variables. See Section 6.2.

- Tool for sensitivity analysis (see Section 7.5).

Version 3.3

- Handling of **categorical variables** for MIXED VARIABLE PROBLEMS (MVP). See Section 7.1.

Version 3.2

- VARIABLE NEIGHBORHOOD SEARCH (VNS) described in Section 7.6.

- **Installers** for `X` systems.

- **Help on parameters** included in the executable: the command 'nomad -h keyword' displays help on the parameters related to `keyword`. Typing only 'nomad -h' or 'nomad -help' displays all the available help: a complete description of all parameters. Also, 'nomad -i' or 'nomad -info' displays information on the current release, and 'nomad -v' displays the current version.

Version 3.1

- **Bi-objective optimization**: see Section 7.2.

- **Periodic variables**: if some variable are periodic, this may be indicated via parameter `PERIODIC_VARIABLE`. Bounds must be defined for these variables. The MADS algorithm adapted to periodic variables is described in [22].

- **Groups of variables** can be defined with the parameter `VARIABLE_GROUP`. At every MADS poll, different directions will be generated for each group. For example, for a location problem, if groups correspond to spatial objects, these will be moved one at a time.

A.6   Future versions

Future algorithmic developments include:

- MULTI-MADS: multi-objective variant of MADS [26], with 3 and more objective functions.

- Improving BIMADS algorithm when feasible solutions are difficult to find.

- Improving the ROBUSTMADS algorithm and develop ROBUSTMADS with constraints.

- Improving parallel versions of NOMAD to handle large range of CPU available.

- Adding ways to account for partial derivative information (greybox instead of blackbox).

Appendix B

Developer parameters

A set of developer parameters are available in the table below for fine tuning algorithmic settings. Additional information on each parameter is available by typing `$NOMAD_HOME/bin/nomad -d PARAM_NAME`.

Please note that the '`-d PARAM_NAME`' option is required which is different than the '`-h PARAM_NAME`' option required for other parameters.

name	arguments	description	default
EPSILON	real	precision on reals	1E-13
INITIAL_MESH_INDEX	integer	initial mesh index for SMESH ℓ_0 [7]	0
MODEL_EVAL_SORT_CAUTIOUS	bool	if the model ordering strategy is cautious	no
MODEL_SEARCH_MAX_TRIAL_PTS	integer	limit on the number of trial points for one model search	10
MODEL_NP1_QUAD_EPSILON	real in $]0;1[$	truncated unit hypercube $]\epsilon;1[^n$ in quad model optimization	0.01
MODEL_SEARCH_PROJ_TO_MESH	bool	if model search trial points are projected to the mesh	yes
MODEL_QUAD_MAX_Y_SIZE	integer	sup. limit on the size of interpolation sets for quadratic models	500
MODEL_QUAD_MIN_Y_SIZE	integer or string 'N+1'	inf. limit on the size of interpolation sets for quadratic models	N+1
MODEL_QUAD_RADIUS_FACTOR	real	quadratic model search radius factor	2.0
MODEL_QUAD_USE_WP	bool	enable the strategy to maintain well-poisedness with quadratic models	no
MULTI_FORMULATION	string	how to compute one value from two objectives	PRODUCT or DIST_L2
MULTI_USE_DELTA_CRIT	bool	use stopping criterion based on δ measure	no
OPPORTUNISTIC_LUCKY_EVAL	bool	parameter for opportunistic strategy	none
OPPORTUNISTIC_MIN_F_IMPRVMT	real	parameter for opportunistic strategy	none
OPPORTUNISTIC_MIN_NB_SUCCESS	integer	parameter for opportunistic strategy	none
OPT_ONLY_SGTE	bool	minimize only with surrogates	no
ROBUST_MADS	bool	use the RobustMads algorithm for smoothing the objective function [21]	no
ROBUST_MADS_STANDARD_DEV_FACTOR	positive real	standard deviation factor in the robust mads	2
SEC_POLL_DIR_TYPE	see 4.2.1	type of directions for the secondary poll	see 4.2.1

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General index

Index of NOMAD parameters