OPHELIA Library
Reference manual

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Contents

Chapter 1

Introduction

Ophelia stands for "Optimization and Harmless Estimation Library for AMLET". The painting "Ophelia" of the front cover is due to Arthur Hughes in 1865.

The library is designed to be install on standard UNIX-like system, so that it is sufficient to use the following commands sequence:

```
./configure
make
make install
```

Optimization compilation options can be specified as arguments of `configure`, for instance:

```
./configure CFLAGS=''-O3 -funroll-loops'' FFLAGS="-O2"
```

You can regenerate the tools with command

```
./bootstrap
```

1.1 BLAS library

`Ophelia` make heavy use of `CBlas` routines, the C version of `Blas` (`http://www.netlib.org/blas`). Many implementations exist, most of them proprietary and restricited to some specific architectures. We only review three open-source implementations: GotoBlas2, GSL Blas, and ATLAS

1.1.1 GotoBlas2

GotoBlas2, available at `http://www.tacc.utexas.edu/tacc-projects/gotoblas2`, is a Blas implementation proposed by the University of Texas

at Austin. Praised as one of the best implementations, it has been released under BSD license in 2010. We therefore strongly recommend its use, and Ophelia is compiled by default with GotoBlas if detected. A local copy is hosted at `http://amlet.slashbin.net`, that has been tested on Arch Linux, Fedora 7, SuSE 11.3, and Mac OS X 10.6.8. On Arch Linux, the compilation required a slight modification of the script `f_check`, obtained by changing `($flags =~ /^\-l/)` with `($flags =~ /^\-l[a-z,A-Z]/)`.

1.1.2 GSL CBlas

GSL (`"http://www.gnu.org/software/gsl/"`) Blas is supported only for convenience reasons, as it is available as a package on all the major distributions. The GPL is however incompatible with OSL, used for many parts of the software. However, Ophelia cannot be viewed as a derived work of GSL CBlas as the code can be compiled without any modifications with other CBlas implementations.

1.1.3 ATLAS

`ATLAS` (`"http://math-atlas.sourceforge.net/"`) is another free implementation of Blas, far better than the GSL one, but which present various issues during the installation process. `Ophelia` will try to detect ATLAS is neither GotoBLAS2 nor GSL CBlas have been found. Note however the you have to install ATLAS as shared libraries in order to be able to run the code.

Chapter 2

Unconstrained optimization

We consider the general problem

$$\min_{x \in \mathcal{R}^n} f(x). \tag{2.1}$$

2.1 Linesearch methods

BFGS Linesearch

2.2 Trust-region methods

2.2.1 Unconstrained optimization

2.3 Hessian approximations

While the gradient $\nabla f(x)$ usually must be known accurately in minimization algorithms, we often can rely on approximations of the Hessian $\nabla^2 f(x)$. This is especially appealing since finite or central differences require $O(n^2)$ function evaluations, which is prohibitive in many applications. In this section, we will focus on traditional secant updates, by focusing on their definitions, but not on the underlying convergence theory. We refer the reader interested in such issues to Chapter 8 of Dennis and Schnabel [2].

Reefering to the original problem 2.1, suppose that we have just taken a step from x_c to x_+. Following Dennis and Schnabel, we consider the Hessian as the derivative matrix of the nonlinear equations system $\nabla f(x) = 0$. The secant equation for the unconstrained minimization problem is

$$H_+ s_c = y_c, \tag{2.2}$$

where

$$s_c = x_+ - x_c,$$
$$y_c = \nabla f(x_+) - \nabla f(x_c).$$

Since the Hessian of some function is symmetric, we seek an H_+ that satisfies $H_+ = H_+^T$ as well as (2.2). The first secant update successfully used in the litterature is the symmetric secand update

BFGS

A popular approximation is the BFGS (Broyden, Fletcher, Goldfarb and Shanno):

$$B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^t d_k} + \frac{B_k d_k (B_k d_k)^T}{d_k^T B_k d_k},$$

where $y_k = \nabla_x f(x_{k+1}) - \nabla_x f(x_k)$.

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2.3.1 Trust-region radius update

Initial trust-region radius

Various options again exist to choose the initial trust-region as well as to update it.

The initialization strategy can be defined by setting the `radius_init` element of the `BTR` structure to the desired user's function, or to NULL, if no initialization has to be performed. In this case, the initial trust-region radius is affected to `BTR_INITIAL_DELTA`, defined in the file `defaults.h`.

The default behaviour of the algorithm sets the initial trust-region to $\|\nabla f(x_0)\|$, as described by Lin and More [3], while more advanced strategies exist. On the first iteration, the predicted step is used to compute a more reasonable trust-region radius, using the formula:

$$\Delta := \min\{\Delta, \|s_0\|\}.$$

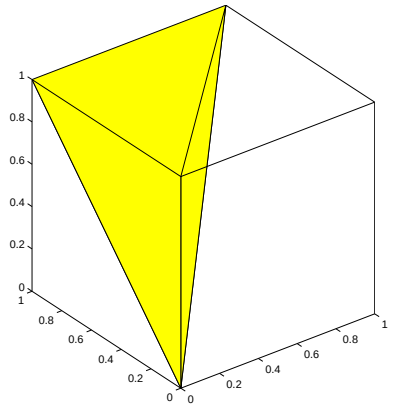
Chapter 3

Constrained optimisation

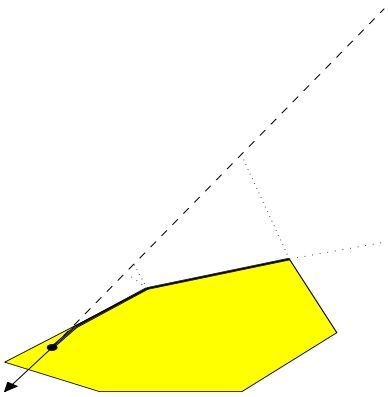
Projection methods

We consider the problem

$$\min_{x \in \mathcal{C}} f(x),$$



the order simplex in 3D



the projected path

3.1 Stopping criteria

3.1.1 Unconstrained optimisation

Relative gradient. Dennis and Schnabel [2], Page 160.

$$\max_i \frac{\nabla f(x)_i \max\{|x_i|, typ\ x_i\}}{\max\{|f(x)|, typ\ f\}},$$

where x_i is the i^{th} component of the vector x.

```
double nlp_relative_gradient(double val, double *x, double *grad,
                             double *typx, int n, double typf)
```

3.1.2 Constrained optimisation

Projection methods for trust-region methods

We use the criterion presented in Conn et al. [1], Section 12.1:

$$\|P[x - \nabla f(x)] - x\|_2 < \epsilon.$$

```
int btr_constrained_projection_stopping_test(BTR *btr, double rho)
```

$$\max_i \frac{(P[x - \nabla f(x)] - x)_i \max\{|x_i|, typ\ x_i\}}{\max\{|f(x)|, f(typ\ f\}},$$

where x_i is the i^{th} component of the vector x.

3.1.3 Specific projection algorithms

Isotonic regression

Isotonic regression (IR) involves finding a weighted least-squares fit $x \in \mathbb{R}^n$ to a vector $a \in \mathbb{R}^n$ with weights vector $w \in \mathbb{R}^n$ subject to a set of monotonicity constraints giving a simple or partial order over the variables.

Chapter 4

Metaheuristics methods

While some metaheuristics algorithms are proposed, it should be stressed that the library does not focus on such methods, and their support is therefore very limited.

4.1 Simulated annealing

```
NlpSa *nlp_sa_new();
```

Overview

Appendix A

Basic analysis

A.1 Banach spaces

A metric space is an ordered pair (M, d) where M is a set and d is a metric on M, that is, a function

$$d : M \times M \to \mathbb{R}$$

such that, for any x, y and z in M,

1. $d(x, y) \geq 0$;
2. $d(x, y) = 0$ if and only if $x = y$;
3. $d(x, y) = d(y, x)$;
4. $d(x, z) \leq d(x, y) + d(y, z)$.

The first condition follows from the other three, since:

$$2d(x, y) = d(x, y) + d(y, x) \geq d(x, x) = 0.$$

A more compact but equivalent definition replaces the above four axioms by the following two:

1. $d(x, y) = 0$ if and only if $x = y$;
2. $d(x, z) \leq d(x, y) + d(z, y)$.

The function d is also called distance function or simply distance. Often d is omitted and one just writes M for a metric space if it is clear from the context what metric is used.

A metric space M is said to be complete (or Cauchy) if every Cauchy sequence of points in M has a limit that is also in M or alternatively if every Cauchy sequence in M converges in M.

A seminormed vector space is a pair (V, p) where V is a vector space and p a seminorm on V. A normed vector space is a pair $(V, \|\cdot\|)$ where V is a vector space and $\|\cdot\|$ a norm on V. We often omit p or $\|\cdot\|$ and just write V for a space if it is clear from the context what (semi)norm we are using.

A Banach space is complete normed vector space. The familiar Euclidean spaces $\mathbb{R}^n$ and $\mathbb{C}^n$, where the Euclidean norm of $x = (x_1, \ldots, x_n)$ is given by

$$\|x\| = \sqrt{\sum_{i=1}^{n} x_i^2},$$

are Banach spaces.

A.2 Topological spaces

A topological space is a set X together with T, a collection of subsets of X, satisfying the following axioms:

1. The empty set and X are in T.
2. The union of any collection of sets in T is also in T.
3. The intersection of any finite collection of sets in T is also in T.

A topological space is called separable if it contains a countable dense subset; that is, there exists a sequence $\left\{_{x_n}\right\}_{n=1}^{\infty}\}$ of elements of the space such that every nonempty open subset of the space contains at least one element of the sequence.

Appendix B

License

All of the code is placed under the OSL. v2.1.

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[3] Chih-Jen Lin and Jorge J. Moré. Newton's method for large bound-constrained optimization problems. *SIAM Journal on Optimization*, 9(4):1100–1127, 1999.

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