DFO-LS Documentation

Release 1.3.0

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CONTENTS:

1 Installing DFO-LS					
	1.1	Requirements	3		
	1.2	Installation using conda	3		
	1.3	Installation using pip	3		
	1.4	Manual installation	4		
	1.5	Testing	4		
	1.6	Uninstallation	5		
2	Over	view	7		
	2.1	When to use DFO-LS	7		
	2.2	Parameter Fitting	7		
	2.3	Solving Nonlinear Systems of Equations	8		
	2.4	Details of the DFO-LS Algorithm	9		
	2.5	References	9		
3	Heine	g DFO-LS	11		
J	3.1		11		
	3.2	•	11		
	3.3		12		
	3.4		13		
	3.5		14		
	3.6	e i	16		
	3.7		17		
	3.8		1 <i>7</i> 19		
	3.9		1 <i>)</i> 21		
	3.10		21 22		
4		8	23		
	4.1	8	23		
	4.2		23		
	4.3		24		
	4.4		24		
	4.5	\mathbf{J}	24		
	4.6	$\boldsymbol{\mathcal{E}}$	24		
	4.7		25		
	4.8		25		
	4.9	ϵ	25		
	4.10	1	25		
	4.11		26		
	4.12	Dykstra's Algorithm	27		

Bi	Bibliography								
8	Ackn	nowledgements	35						
	7.2	Contributors	33						
7	Cont 7.1	ributors Main author	33						
_	~								
	6.10	Version 1.3.0 (8 Nov 2021)	32						
	6.9	Version 1.2.3 (1 Jun 2021)	32						
	6.8	Version 1.2.2 (26 Feb 2021)	32						
	6.7	Version 1.2.1 (13 Feb 2020)	32						
	6.6	Version 1.1.1 (5 Apr 2019)	32						
	6.4 6.5	Version 1.1 (16 Jan 2019)	31 32						
	6.3	Version 1.0.2 (20 Jun 2018)	31						
	6.2	Version 1.0.1 (20 Feb 2018)	31						
	6.1	Version 1.0 (6 Feb 2018)	31						
6	Versi	on History	31						
	5.5	Algorithm Progress	30						
	5.4	Iteration Count	30						
	5.3	Model Interpolation	30						
	5.2	Trust Region							
5	Diagi 5.1	nostic Information Current Iterate	29 29						
		References							
	1 12	Checking Matrix Rank	27						

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DFO-LS is a flexible package for finding local solutions to nonlinear least-squares minimization problems (with optional constraints), without requiring any derivatives of the objective. DFO-LS stands for Derivative-Free Optimizer for Least-Squares.

That is, DFO-LS solves

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} & f(x) := \sum_{i=1}^m r_i(x)^2 \\ & \text{s.t.} & x \in C \\ & a \leq x \leq b \end{aligned}$$

The constraint set C is the intersection of multiple convex sets provided as input by the user. All constraints are non-relaxable (i.e. DFO-LS will never ask to evaluate a point that is not feasible).

Full details of the DFO-LS algorithm are given in our papers:

- C. Cartis, J. Fiala, B. Marteau and L. Roberts, Improving the Flexibility and Robustness of Model-Based Derivative-Free Optimization Solvers, ACM Transactions on Mathematical Software, 45:3 (2019), pp. 32:1-32:41 [preprint].
- Hough, M. and Roberts, L., Model-Based Derivative-Free Methods for Convex-Constrained Optimization, *arXiv* preprint arXiv:2111.05443, (2021).

DFO-LS is a more flexible version of DFO-GN.

If you are interested in solving general optimization problems (without a least-squares structure), you may wish to try Py-BOBYQA, which has many of the same features as DFO-LS.

DFO-LS is released under the GNU General Public License. Please contact NAG for alternative licensing.

CONTENTS: 1

2 CONTENTS:

CHAPTER

ONE

INSTALLING DFO-LS

1.1 Requirements

DFO-LS requires the following software to be installed:

• Python 2.7 or Python 3 (http://www.python.org/)

Additionally, the following python packages should be installed (these will be installed automatically if using *pip*, see *Installation using pip*):

- NumPy 1.11 or higher (http://www.numpy.org/)
- SciPy 0.18 or higher (http://www.scipy.org/)
- Pandas 0.17 or higher (http://pandas.pydata.org/)

Optional package: DFO-LS versions 1.2 and higher also support the trustregion package for fast trust-region subproblem solutions. To install this, make sure you have a Fortran compiler (e.g. gfortran) and NumPy installed, then run pip install trustregion. You do not have to have trustregion installed for DFO-LS to work, and it is not installed by default.

1.2 Installation using conda

DFO-LS can be directly installed in Anaconda environments using conda-forge:

```
$ conda install -c conda-forge dfo-ls
```

1.3 Installation using pip

For easy installation, use pip (http://www.pip-installer.org/) as root:

```
.. code-block:: bash
$ [sudo] pip install DFO-LS
```

or alternatively *easy_install*:

```
.. code-block:: bash
$ [sudo] easy_install DFO-LS
```

If you do not have root privileges or you want to install DFO-LS for your private use, you can use:

```
.. code-block:: bash

$ pip install --user DFO-LS
```

which will install DFO-LS in your home directory.

Note that if an older install of DFO-LS is present on your system you can use:

```
.. code-block:: bash
$ [sudo] pip install --upgrade DFO-LS
```

to upgrade DFO-LS to the latest version.

1.4 Manual installation

Alternatively, you can download the source code from Github and unpack as follows:

```
$ git clone https://github.com/numericalalgorithmsgroup/dfols
$ cd dfols
```

DFO-LS is written in pure Python and requires no compilation. It can be installed using:

```
$ [sudo] pip install .
```

If you do not have root privileges or you want to install DFO-LS for your private use, you can use:

```
$ pip install --user .
```

instead.

To upgrade DFO-LS to the latest version, navigate to the top-level directory (i.e. the one containing setup.py) and rerun the installation using pip, as above:

```
$ git pull
$ [sudo] pip install . # with admin privileges
```

1.5 Testing

If you installed DFO-LS manually, you can test your installation by running:

```
$ python setup.py test
```

Alternatively, the HTML documentation provides some simple examples of how to run DFO-LS.

1.6 Uninstallation

If DFO-LS was installed using *pip* you can uninstall as follows:

```
$ [sudo] pip uninstall DFO-LS
```

If DFO-LS was installed manually you have to remove the installed files by hand (located in your python site-packages directory).

1.6. Uninstallation 5

CHAPTER

TWO

OVERVIEW

2.1 When to use DFO-LS

DFO-LS is designed to solve the nonlinear least-squares minimization problem (with optional convex constraints).

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} \quad f(x) := \sum_{i=1}^m r_i(x)^2 \\ & \text{s.t.} \quad x \in C \\ & \quad a < x < b \end{aligned}$$

We call f(x) the objective function and $r_i(x)$ the residual functions (or simply residuals). C is the intersection of multiple convex sets given as input by the user.

DFO-LS is a *derivative-free* optimization algorithm, which means it does not require the user to provide the derivatives of f(x) or $r_i(x)$, nor does it attempt to estimate them internally (by using finite differencing, for instance).

There are two main situations when using a derivative-free algorithm (such as DFO-LS) is preferable to a derivative-based algorithm (which is the vast majority of least-squares solvers).

If the residuals are noisy, then calculating or even estimating their derivatives may be impossible (or at least very inaccurate). By noisy, we mean that if we evaluate $r_i(x)$ multiple times at the same value of x, we get different results. This may happen when a Monte Carlo simulation is used, for instance, or $r_i(x)$ involves performing a physical experiment.

If the residuals are expensive to evaluate, then estimating derivatives (which requires n evaluations of each $r_i(x)$ for every point of interest x) may be prohibitively expensive. Derivative-free methods are designed to solve the problem with the fewest number of evaluations of the objective as possible.

However, if you have provide (or a solver can estimate) derivatives of $r_i(x)$, then it is probably a good idea to use one of the many derivative-based solvers (such as one from the SciPy library).

2.2 Parameter Fitting

A very common problem in many quantitative disciplines is fitting parameters to observed data. Typically, this means that we have developed a model for some process, which takes a vector of (known) inputs obs $\in \mathbb{R}^N$ and some model parameters $x = (x_1, \dots, x_n) \in \mathbb{R}^n$, and computes a (predicted) quantity of interest $y \in \mathbb{R}$:

$$y = model(obs, x)$$

For this model to be useful, we need to determine a suitable choice for the parameters x, which typically cannot be directly observed. A common way of doing this is to calibrate from observed relationships.

Suppose we have some observations of the input-to-output relationship. That is, we have data

$$(obs_1, y_1), \ldots, (obs_m, y_m)$$

Then, we try to find the parameters x which produce the best possible fit to these observations by minimizing the sum-of-squares of the prediction errors:

$$\min_{x \in \mathbb{R}^n} \quad f(x) := \sum_{i=1}^m (y_i - \text{model}(\text{obs}_i, x))^2$$

which is in the least-squares form required by DFO-LS.

As described above, DFO-LS is a particularly good choice for parameter fitting when the model has noise (e.g. Monte Carlo simulation) or is expensive to evaluate.

2.3 Solving Nonlinear Systems of Equations

Suppose we wish to solve the system of nonlinear equations: find $x \in \mathbb{R}^n$ satisfying

$$r_1(x) = 0$$

$$r_2(x) = 0$$

$$\vdots$$

$$r_m(x) = 0$$

Such problems can have no solutions, one solution, or many solutions (possibly infinitely many). Often, but certainly not always, the number of solutions depends on whether there are more equations or unknowns: if m < n we say the system is underdetermined (and there are often multiple solutions), if m = n we say the system is square (and there is often only one solution), and if m > n we say the system is overdetermined (and there are often no solutions).

This is not always true – there is no solution to the underdetermined system when m=1 and n=2 and we choose $r_1(x)=\sin(x_1+x_2)-2$, for example. Similarly, if we take n=1 and $r_i(x)=i(x-1)(x-2)$, we can make m as large as we like while keeping x=1 and x=2 as solutions (to the overdetermined system).

If no solution exists, it makes sense to instead search for an x which approximately satisfies each equation. A common way to do this is to minimize the sum-of-squares of the left-hand-sides:

$$\min_{x \in \mathbb{R}^n} \quad f(x) := \sum_{i=1}^m r_i(x)^2$$

which is the form required by DFO-LS.

If a solution does exist, then this formulation will also find this (where we will get f = 0 at the solution).

Which solution? DFO-LS, and most similar software, will only find one solution to a set of nonlinear equations. Which one it finds is very difficult to predict, and depends very strongly on the point where the solver is started from. Often it finds the closest solution, but there are no guarantees this will be the case. If you need to find all/multiple solutions for your problem, consider techniques such as deflation.

2.4 Details of the DFO-LS Algorithm

DFO-LS is a type of trust-region method, a common category of optimization algorithms for nonconvex problems. Given a current estimate of the solution x_k , we compute a model which approximates the objective $m_k(s) \approx f(x_k + s)$ (for small steps s), and maintain a value $\Delta_k > 0$ (called the trust region radius) which measures the size of s for which the approximation is good.

At each step, we compute a trial step s_k designed to make our approximation $m_k(s)$ small (this task is called the *trust region subproblem*). We evaluate the objective at this new point, and if this provided a good decrease in the objective, we take the step $(x_{k+1} = x_k + s_k)$, otherwise we stay put $(x_{k+1} = x_k)$. Based on this information, we choose a new value Δ_{k+1} , and repeat the process.

In DFO-LS, we construct our approximation $m_k(s)$ by interpolating a linear approximation for each residual $r_i(x)$ at several points close to x_k . To make sure our interpolated model is accurate, we need to regularly check that the points are well-spaced, and move them if they aren't (i.e. improve the geometry of our interpolation points).

A complete description of the DFO-LS algorithm is given in our papers [CFMR2018] and [HR2021].

2.5 References

CHAPTER

THREE

USING DFO-LS

This section describes the main interface to DFO-LS and how to use it.

3.1 Nonlinear Least-Squares Minimization

DFO-LS is designed to solve the local optimization problem

$$\min_{x \in \mathbb{R}^n} \quad f(x) := \sum_{i=1}^m r_i(x)^2$$

where the set C is an optional non-empty, closed and convex constraint set. The constraints are non-relaxable (i.e. DFO-LS will never ask to evaluate a point that is not feasible).

DFO-LS iteratively constructs an interpolation-based model for the objective, and determines a step using a trust-region framework. For an in-depth technical description of the algorithm see the papers [CFMR2018] and [HR2021].

3.2 How to use DFO-LS

The main interface to DFO-LS is via the function solve

```
soln = dfols.solve(objfun, x0)
```

The input objfun is a Python function which takes an input $x \in \mathbb{R}^n$ and returns the vector of residuals $[r_1(x) \cdots r_m(x)] \in \mathbb{R}^m$. Both the input and output of objfun must be one-dimensional NumPy arrays (i.e. with x.shape == (n,) and objfun(x).shape == (m,)).

The input x0 is the starting point for the solver, and (where possible) should be set to be the best available estimate of the true solution $x_{min} \in \mathbb{R}^n$. It should be specified as a one-dimensional NumPy array (i.e. with x0. shape == (n,)). As DFO-LS is a local solver, providing different values for x0 may cause it to return different solutions, with possibly different objective values.

The output of dfols.solve is an object containing:

- soln.x an estimate of the solution, $x_{min} \in \mathbb{R}^n$, a one-dimensional NumPy array.
- soln.resid the vector of residuals at the calculated solution, $[r_1(x_{min}) \cdots r_m(x_{min})]$, a one-dimensional NumPy array.
- ullet soln.f the objective value at the calculated solution, $f(x_{min})$, a Float.
- soln.jacobian an estimate of the Jacobian matrix of first derivatives of the residuals, $J_{i,j} \approx \partial r_i(x_{min})/\partial x_j$, a NumPy array of size $m \times n$.

- soln.nf the number of evaluations of objfun that the algorithm needed, an Integer.
- soln.nx the number of points x at which objfun was evaluated, an Integer. This may be different to soln.nf if sample averaging is used.
- soln.nruns the number of runs performed by DFO-LS (more than 1 if using multiple restarts), an Integer.
- soln.flag an exit flag, which can take one of several values (listed below), an Integer.
- soln.msg a description of why the algorithm finished, a String.
- soln.diagnostic_info a table of diagnostic information showing the progress of the solver, a Pandas DataFrame.

The possible values of soln.flag are defined by the following variables:

- soln.EXIT_SUCCESS DFO-LS terminated successfully (the objective value or trust region radius are sufficiently small).
- soln.EXIT_MAXFUN_WARNING maximum allowed objective evaluations reached. This is the most likely return value when using multiple restarts.
- soln.EXIT_SLOW_WARNING maximum number of slow iterations reached.
- soln.EXIT_FALSE_SUCCESS_WARNING DFO-LS reached the maximum number of restarts which decreased the objective, but to a worse value than was found in a previous run.
- soln.EXIT_TR_INCREASE_WARNING model increase when solving the trust region subproblem with multiple arbitrary constraints.
- soln.EXIT INPUT ERROR error in the inputs.
- soln.EXIT_TR_INCREASE_ERROR error occurred when solving the trust region subproblem.
- soln.EXIT_LINALG_ERROR linear algebra error, e.g. the interpolation points produced a singular linear system.

These variables are defined in the soln object, so can be accessed with, for example

```
if soln.flag == soln.EXIT_SUCCESS:
    print("Success!")
```

3.3 Optional Arguments

The solve function has several optional arguments which the user may provide:

```
dfols.solve(objfun, x0, args=(), bounds=None, projections=[], npt=None, 

→rhobeg=None,

rhoend=1e-8, maxfun=None, nsamples=None,

user_params=None, objfun_has_noise=False,

scaling_within_bounds=False,

do_logging=True, print_progress=False)
```

These arguments are:

- args a tuple of extra arguments passed to the objective function.
- bounds a tuple (lower, upper) with the vectors a and b of lower and upper bounds on x (default is $a_i = -10^{20}$ and $b_i = 10^{20}$). To set bounds for either lower or upper, but not both, pass a tuple (lower, None) or (None, upper).

- projections a list [f1, f2, ..., fn] of functions that each take as input a point x and return a new point y. The new point y should be given by the projection of x onto a closed convex set. The intersection of all sets corresponding to a function must be non-empty.
- npt the number of interpolation points to use (default is len(x0)+1). If using restarts, this is the number of points to use in the first run of the solver, before any restarts (and may be optionally increased via settings in user_params).
- rhobeg the initial value of the trust region radius (default is $0.1 \max(\|x_0\|_{\infty}, 1)$, or 0.1 if scaling within bounds).
- rhoend minimum allowed value of trust region radius, which determines when a successful termination occurs (default is 10^{-8}).
- maxfun the maximum number of objective evaluations the algorithm may request (default is $\min(100(n+1),1000)$).
- nsamples a Python function nsamples (delta, rho, iter, nrestarts) which returns the number of times to evaluate objfun at a given point. This is only applicable for objectives with stochastic noise, when averaging multiple evaluations at the same point produces a more accurate value. The input parameters are the trust region radius (delta), the lower bound on the trust region radius (rho), how many iterations the algorithm has been running for (iter), and how many restarts have been performed (nrestarts). Default is no averaging (i.e. nsamples (delta, rho, iter, nrestarts) = 1).
- user_params a Python dictionary { 'param1': val1, 'param2':val2, ...} of optional parameters. A full list of available options is given in the next section *Advanced Usage*.
- objfun_has_noise a flag to indicate whether or not objfun has stochastic noise; i.e. will calling objfun(x) multiple times at the same value of x give different results? This is used to set some sensible default parameters (including using multiple restarts), all of which can be overridden by the values provided in user_params.
- scaling_within_bounds a flag to indicate whether the algorithm should internally shift and scale the entries of x so that the bounds become $0 \le x \le 1$. This is useful is you are setting bounds and the bounds have different orders of magnitude. If scaling_within_bounds=True, the values of rhobeg and rhoend apply to the *shifted* variables.
- do_logging a flag to indicate whether logging output should be produced. This is not automatically visible unless you use the Python logging module (see below for simple usage).
- print_progress a flag to indicate whether to print a per-iteration progress log to terminal.

In general when using optimization software, it is good practice to scale your variables so that moving each by a given amount has approximately the same impact on the objective function. The scaling_within_bounds flag is designed to provide an easy way to achieve this, if you have set the bounds lower and upper.

3.4 A Simple Example

Suppose we wish to minimize the Rosenbrock test function:

$$\min_{(x_1, x_2) \in \mathbb{R}^2} \quad 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

This function has exactly one local minimum $f(x_{min}) = 0$ at $x_{min} = (1, 1)$. We can write this as a least-squares problem as:

$$\min_{(x_1, x_2) \in \mathbb{R}^2} \ [10(x_2 - x_1^2)]^2 + [1 - x_1]^2$$

A commonly-used starting point for testing purposes is $x_0 = (-1.2, 1)$. The following script shows how to solve this problem using DFO-LS:

```
# DFO-LS example: minimize the Rosenbrock function
from __future__ import print_function
import numpy as np
import dfols

# Define the objective function
def rosenbrock(x):
    return np.array([10.0 * (x[1] - x[0] ** 2), 1.0 - x[0]])

# Define the starting point
x0 = np.array([-1.2, 1.0])

# Call DFO-LS
soln = dfols.solve(rosenbrock, x0)

# Display output
print(soln)
```

Note that DFO-LS is a randomized algorithm: in its first phase, it builds an internal approximation to the objective function by sampling it along random directions. In the code above, we set NumPy's random seed for reproducibility over multiple runs, but this is not required. The output of this script, showing that DFO-LS finds the correct solution, is

This and all following problems can be found in the examples directory on the DFO-LS Github page.

3.5 Adding Bounds and More Output

We can extend the above script to add constraints. To add bound constraints alone, we can add the lines

```
# Define bound constraints (lower <= x <= upper)
lower = np.array([-10.0, -10.0])
upper = np.array([0.9, 0.85])

# Call DFO-LS (with bounds)
soln = dfols.solve(rosenbrock, x0, bounds=(lower, upper))</pre>
```

DFO-LS correctly finds the solution to the constrained problem:

```
****** DFO-LS Results *****
Solution xmin = [0.9 0.81]
Residual vector = [3.10862447e-14 1.00000000e-01]
Objective value f(xmin) = 0.01
Needed 58 objective evaluations (at 58 points)
Approximate Jacobian = [[-1.79999999e+01 9.99999998e+00]

(continues on next page)
```

However, we also get a warning that our starting point was outside of the bounds:

```
RuntimeWarning: x0 above upper bound, adjusting
```

DFO-LS automatically fixes this, and moves x_0 to a point within the bounds, in this case $x_0 = (-1.2, 0.85)$.

We can also get DFO-LS to print out more detailed information about its progress using the logging module. To do this, we need to add the following lines:

```
import logging
logging.basicConfig(level=logging.INFO, format='%(message)s')
# ... (call dfols.solve)
```

And for the simple bounds example we can now see each evaluation of objfun:

If we wanted to save this output to a file, we could replace the above call to logging.basicConfig() with

If you have logging for some parts of your code and you want to deactivate all DFO-LS logging, you can use the optional argument do_logging=False in dfols.solve().

An alternative option available is to get DFO-LS to print to terminal progress information every iteration, by setting the optional argument print_progress=True in dfols.solve(). If we do this for the above example, we get

```
Run
    Iter
             Obj
                       Grad
                                Delta
                                           rho
                                                   Evals
1
      1
           1.43e+01 1.61e+02 1.20e-01 1.20e-01
                                                     3
           4.35e+00 3.77e+01 4.80e-01 1.20e-01
                                                     4
1
      2.
      3
           4.35e+00 3.77e+01 6.00e-02 1.20e-02
                                                     4
1
1
     55
           1.00e-02 2.00e-01 1.50e-08 1.00e-08
                                                    56
1
     56
           1.00e-02 2.00e-01 1.50e-08
                                        1.00e-08
                                                    57
```

3.6 Handling Arbitrary Convex Constraints

DFO-LS can also handle more general constraints where they can be written as the intersection of finitely many convex sets. For example, the below code minimizes the Rosenbrock function subject to a constraint set given by the intersection of two convex sets. Note the intersection of the user-provided convex sets must be non-empty.

```
DFO-LS example: minimize the Rosenbrock function with arbitrary convex_
This example defines two functions pball(x) and pbox(x) that project onto,
box constraint sets respectively. It then passes both these functions to the
\hookrightarrow DFO-LS
solver so that it can find a constrained minimizer to the Rosenbrock
\hookrightarrow function.
Such a minimizer must lie in the intersection of constraint sets.
⇔corresponding to
projection functions pball(x) and pbox(x). The description of the problem is_
→as follows:
   min rosenbrock(x)
    s.t.
        -2 <= x[0] <= 1.1,
       1.1 <= x[1] <= 3,
       norm(x-c) <= 0.4
where c = [0.7, 1.5] is the centre of the ball.
from __future__ import print_function
import numpy as np
import dfols
# Define the objective function
def rosenbrock(x):
    return np.array([10.0 * (x[1] - x[0] ** 2), 1.0 - x[0]])
# Define the starting point
x0 = np.array([-1.2, 1])
Define ball projection function
Projects the input x onto a ball with
centre point (0.7,1.5) and radius 0.4.
def pball(x):
   c = np.array([0.7, 1.5]) # ball centre
   r = 0.4 \# ball radius
   return c + (r/np.max([np.linalg.norm(x-c),r]))*(x-c)
r \cdot r \cdot r
Define box projection function
Projects the input x onto a box
such that -2 \ll x[0] \ll 0.9 and
1.1 <= x[1] <= 3.
Note: One could equivalently add bound
```

```
constraints as a separate input to the solver
instead.
'''

def pbox(x):
    1 = np.array([-2, 1.1]) # lower bound
    u = np.array([0.9, 3]) # upper bound
    return np.minimum(np.maximum(x,1), u)

# For optional extra output details
import logging
logging.basicConfig(level=logging.DEBUG, format='%(message)s')

# Call DFO-LS
soln = dfols.solve(rosenbrock, x0, projections=[pball,pbox])

# Display output
print(soln)
```

Note that for bound constraints one can choose to either implement them by defining a projection function as above, or by passing the bounds as input like in the example from the section on adding bound constraints.

DFO-LS correctly finds the solution to this constrained problem too. Note that we get a warning because the step computed in the trust region subproblem gave an increase in the model. This is common in the case where multiple constraints are active at the optimal point.

3.7 Example: Noisy Objective Evaluation

As described in *Overview*, derivative-free algorithms such as DFO-LS are particularly useful when objfun has noise. Let's modify the previous example to include random noise in our objective evaluation, and compare it to a derivative-based solver:

```
# DFO-LS example: minimize the noisy Rosenbrock function
from __future__ import print_function
import numpy as np
import dfols

# Define the objective function
def rosenbrock(x):
    return np.array([10.0 * (x[1] - x[0] ** 2), 1.0 - x[0]])

# Modified objective function: add 1% Gaussian noise
def rosenbrock_noisy(x):
```

```
return rosenbrock(x) * (1.0 + 1e-2 * np.random.normal(size=(2,)))
# Define the starting point
x0 = np.array([-1.2, 1.0])
# Set random seed (for reproducibility)
np.random.seed(0)
print("Demonstrate noise in function evaluation:")
for i in range(5):
   print ("objfun(x0) = %s" % str(rosenbrock_noisy(x0)))
print("")
# Call DFO-LS
soln = dfols.solve(rosenbrock_noisy, x0)
# Display output
print(soln)
# Compare with a derivative-based solver
import scipy.optimize as opt
soln = opt.least_squares(rosenbrock_noisy, x0)
print("")
print("** SciPy results **")
print("Solution xmin = %s" % str(soln.x))
print("Objective value f(xmin) = %.10q" % (2.0 * soln.cost))
print("Needed %g objective evaluations" % soln.nfev)
print("Exit flag = %g" % soln.status)
print(soln.message)
```

The output of this is:

```
Demonstrate noise in function evaluation:
objfun(x0) = [-4.4776183 2.20880346]
objfun(x0) = [-4.44306447 2.24929965]
objfun(x0) = [-4.48217255 2.17849989]
objfun(x0) = [-4.44180389 2.19667014]
objfun(x0) = [-4.39545837 2.20903317]
***** DFO-LS Results *****
Solution xmin = [1.
                          1.000000031
Residual vector = [1.59634974e-07 -4.63036198e-09]
Objective value f(xmin) = 2.550476524e-14
Needed 53 objective evaluations (at 53 points)
Approximate Jacobian = [[-1.98196347e+01 9.90335675e+00]
[-1.01941978e+00 4.24991776e-05]]
Exit flag = 0
Success: Objective is sufficiently small
******
** SciPy results **
Solution xmin = [-1.20000087 1.00000235]
Objective value f(xmin) = 23.95535774
Needed 6 objective evaluations
Exit flag = 3
```

```
`xtol` termination condition is satisfied.
```

DFO-LS is able to find the solution with 20 more function evaluations as in the noise-free case. However SciPy's derivative-based solver, which has no trouble solving the noise-free problem, is unable to make any progress.

As noted above, DFO-LS has an input parameter objfun_has_noise to indicate if objfun has noise in it, which it does in this case. Therefore we can call DFO-LS with

```
soln = dfols.solve(rosenbrock_noisy, x0, objfun_has_noise=True)
```

Using this setting, we find the correct solution faster:

3.8 Example: Parameter Estimation/Data Fitting

Next, we show a short example of using DFO-LS to solve a parameter estimation problem (taken from here). Given some observations (t_i, y_i) , we wish to calibrate parameters $x = (x_1, x_2)$ in the exponential decay model

$$y(t) = x_1 \exp(x_2 t)$$

The code for this is:

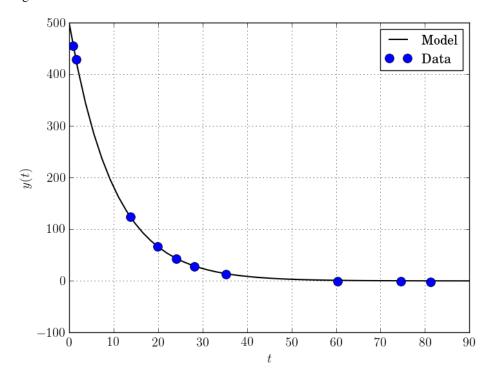
```
# DFO-LS example: data fitting problem
# Originally from:
# https://uk.mathworks.com/help/optim/ug/lsqcurvefit.html
from __future__ import print_function
import numpy as np
import dfols
# Observations
tdata = np.array([0.9, 1.5, 13.8, 19.8, 24.1, 28.2, 35.2,
                  60.3, 74.6, 81.3])
ydata = np.array([455.2, 428.6, 124.1, 67.3, 43.2, 28.1, 13.1,
                  -0.4, -1.3, -1.5
# Model is y(t) = x[0] * exp(x[1] * t)
def prediction_error(x):
    return ydata - x[0] * np.exp(x[1] * tdata)
# Define the starting point
x0 = np.array([100.0, -1.0])
# We expect exponential decay: set upper bound x[1] \le 0
upper = np.array([1e20, 0.0])
```

```
# Call DFO-LS
soln = dfols.solve(prediction_error, x0, bounds=(None, upper))
# Display output
print(soln)
```

The output of this is (noting that DFO-LS moves x_0 to be far away enough from the upper bound)

```
***** DFO-LS Results *****
Solution xmin = [4.98830861e+02 -1.01256863e-01]
Residual vector = [-0.1816709]
                               0.06098397 0.76276301 0.11962354 -0.
\leftrightarrow 26589796 -0.59788814
-1.02611897 -1.5123537 -1.56145452 -1.63266662]
Objective value f(xmin) = 9.504886892
Needed 79 objective evaluations (at 79 points)
Approximate Jacobian = [[-9.12897463e-01 -4.09843514e+02]
[-8.59085679e-01 -6.42808544e+02]
[-2.47252555e-01 -1.70205419e+03]
 [-1.34676365e-01 -1.33017181e+03]
[-8.71355033e-02 -1.04752848e+03]
[-5.75304364e-02 -8.09280752e+02]
[-2.83184867e-02 -4.97239623e+02]
[-2.22992989e-03 -6.70749826e+01]
[-5.24129962e-04 -1.95045269e+01]
[-2.65956876e-04 -1.07858081e+01]]
Exit flag = 0
Success: rho has reached rhoend
*********
```

This produces a good fit to the observations.



To generate this plot, run:

```
# Plot calibrated model vs. observations
ts = np.linspace(0.0, 90.0)
ys = soln.x[0] * np.exp(soln.x[1] * ts)

import matplotlib.pyplot as plt
plt.figure(1)
ax = plt.gca() # current axes
ax.plot(ts, ys, 'k-', label='Model')
ax.plot(tdata, ydata, 'bo', label='Data')
ax.set_xlabel('t')
ax.set_ylabel('y(t)')
ax.legend(loc='upper right')
ax.grid()
plt.show()
```

3.9 Example: Solving a Nonlinear System of Equations

Lastly, we give an example of using DFO-LS to solve a nonlinear system of equations (taken from here). We wish to solve the following set of equations

$$x_1 + x_2 - x_1x_2 + 2 = 0,$$

 $x_1 \exp(-x_2) - 1 = 0.$

The code for this is:

```
# DFO-LS example: Solving a nonlinear system of equations
# Originally from:
# http://support.sas.com/documentation/cdl/en/imluq/66112/HTML/default/
→viewer.htm#imlug_genstatexpls_sect004.htm
from __future__ import print_function
from math import exp
import numpy as np
import dfols
# Want to solve:
\# x1 + x2 - x1*x2 + 2 = 0
  x1 * exp(-x2) - 1 = 0
def nonlinear_system(x):
   return np.array([x[0] + x[1] - x[0] *x[1] + 2,
                     x[0] * exp(-x[1]) - 1.0]
# Warning: if there are multiple solutions, which one
          DFO-LS returns will likely depend on x0!
x0 = np.array([0.1, -2.0])
# Call DFO-LS
soln = dfols.solve(nonlinear_system, x0)
# Display output
print(soln)
```

The output of this is

Here, we see that both entries of the residual vector are very small, so both equations have been solved to high accuracy.

3.10 References

ADVANCED USAGE

This section describes different optional user parameters available in DFO-LS.

In the last section (*Using DFO-LS*), we introduced dfols.solve(), which has the optional input user_params. This is a Python dictionary of user parameters. We will now go through the settings which can be changed in this way. More details are available in the papers [CFMR2018] and [HR2021].

The default values, used if no override is given, in some cases vary depending on whether objfun has stochastic noise; that is, whether evaluating objfun(x) several times at the same x gives the same result or not. Whether or not this is the case is determined by the objfun_has_noise input to dfols.solve() (and not by inspecting objfun, for instance).

4.1 General Algorithm Parameters

- general.rounding_error_constant Internally, all interpolation points are stored with respect to a base point x_b ; that is, we store $\{y_t x_b\}$, which reduces the risk of roundoff errors. We shift x_b to x_k when $\|s_k\| \le \text{const} \|x_k x_b\|$, where 'const' is this parameter. Default is 0.1.
- general.safety_step_thresh Threshold for when to call the safety step, $||s_k|| \le \gamma_S \rho_k$. Default is $\gamma_S = 0.5$.
- general.check_objfun_for_overflow Whether to cap the value of $r_i(x)$ when they are large enough that an OverflowError will be encountered when trying to evaluate f(x). Default is True.

4.2 Logging and Output

- logging.n_to_print_whole_x_vector If printing all function evaluations to screen/log file, the maximum len(x) for which the full vector x should be printed also. Default is 6.
- logging.save_diagnostic_info Flag so save diagnostic information at each iteration. Default is False.
- logging.save_poisedness If saving diagnostic information, whether to include the Λ -poisedness of Y_k in the diagnostic information. This is the most computationally expensive piece of diagnostic information. Default is True.
- logging.save_xk If saving diagnostic information, whether to include the full vector x_k . Default is False.
- logging.save_rk-If saving diagnostic information, whether to include the full vector $[r_1(x_k)\cdots r_m(x_k)]$. The value $f(x_k)$ is always included. Default is False.

4.3 Initialization of Points

- init.random_initial_directions Build the initial interpolation set using random directions (as opposed to coordinate directions). Default as of version 1.2 is False.
- init.random_directions_make_orthogonal If building initial interpolation set with random directions, whether or not these should be orthogonalized. Default is True.
- init.run_in_parallel If using random directions, whether or not to ask for all objfun to be evaluated at all points without any intermediate processing. Default is False.

4.4 Trust Region Management

- tr_radius.etal Threshold for unsuccessful trust region iteration, η_1 . Default is 0.1.
- tr_radius.eta2 Threshold for very successful trust region iteration, η_2 . Default is 0.7.
- tr_radius.gamma_dec Ratio to decrease Δ_k in unsuccessful iteration, γ_{dec} . Default is 0.5 for smooth problems or 0.98 for noisy problems (i.e. objfun_has_noise = True).
- tr_radius.gamma_inc Ratio to increase Δ_k in very successful iterations, γ_{inc} . Default is 2.
- tr_radius.gamma_inc_overline Ratio of $||s_k||$ to increase Δ_k by in very successful iterations, $\overline{\gamma}_{inc}$. Default is 4.
- tr_radius.alpha1 Ratio to decrease ρ_k by when it is reduced, α_1 . Default is 0.1 for smooth problems or 0.9 for noisy problems (i.e. objfun_has_noise = True).
- tr_radius.alpha2 Ratio of ρ_k to decrease Δ_k by when ρ_k is reduced, α_2 . Default is 0.5 for smooth problems or 0.95 for noisy problems (i.e. objfun_has_noise = True).

4.5 Termination on Small Objective Value

- model.abs tol-Tolerance on $f(x_k)$; quit if $f(x_k)$ is below this value. Default is 10^{-12} .
- model.rel_tol Relative tolerance on $f(x_k)$; quit if $f(x_k)/f(x_0)$ is below this value. Default is 10^{-20} .

4.6 Termination on Slow Progress

- slow.history_for_slow History used to determine whether the current iteration is 'slow'. Default is 5.
- slow.thresh_for_slow Threshold for objective decrease used to determine whether the current iteration is 'slow'. Default is 10^{-4} .
- slow.max_slow_iters Number of consecutive slow successful iterations before termination (or restart). Default is 20*len(x0).

4.7 Stochastic Noise Information

- noise.quit_on_noise_level Flag to quit (or restart) if all $f(y_t)$ are within noise level of $f(x_k)$. Default is False for smooth problems or True for noisy problems.
- noise.scale_factor_for_quit Factor of noise level to use in termination criterion. Default is 1.
- noise.multiplicative_noise_level Multiplicative noise level in f. Can only specify one of multiplicative or additive noise levels. Default is None.
- noise.additive_noise_level Additive noise level in f. Can only specify one of multiplicative or additive noise levels. Default is None.

4.8 Interpolation Management

- interpolation.precondition whether or not to scale the interpolation linear system to improve conditioning. Default is True.
- interpolation.throw_error_on_nans whether or not to throw numpy.linalg.LinAlgError if trying to interpolate to NaN objective values. If False, DFO-LS should terminate gracefully with an error flag. Default is False.

4.9 Regression Model Management

- regression.num_extra_steps In successful iterations, the number of extra points (other than accepting the trust region step) to move, useful when $|Y_k| > n+1$ (n is len(x0)). Default is 0.
- regression.increase_num_extra_steps_with_restart The amount to increase regression.num_extra_steps by with each restarts, for instance if increasing the number of points with each restart. Default is 0.
- regression.momentum_extra_steps If moving extra points in successful iterations, whether to use the 'momentum' method. If not, uses geometry-improving steps. Default is False.

4.10 Multiple Restarts

- restarts.use_restarts Whether to do restarts when ρ_k reaches ρ_{end} , or (optionally) when all points are within noise level of $f(x_k)$. Default is False for smooth problems or True for noisy problems.
- restarts.max_unsuccessful_restarts Maximum number of consecutive unsuccessful restarts allowed (i.e.~restarts which did not reduce the objective further). Default is 10.
- restarts.rhoend_scale Factor to reduce ho_{end} by with each restart. Default is 1.
- restarts.use_soft_restarts Whether to use soft or hard restarts. Default is True.
- restarts.soft.num_geom_steps For soft restarts, the number of points to move. Default is 3.
- restarts.soft.move_xk For soft restarts, whether to preserve x_k , or move it to the best new point evaluated. Default is True.
- restarts.increase_npt Whether to increase $|Y_k|$ with each restart. Default is False.
- ullet restarts.increase_npt_amt Amount to increase $|Y_k|$ by with each restart. Default is 1.

- restarts.hard.increase_ndirs_initial_amt Amount to increase growing. ndirs_initial by with each hard restart. To avoid a growing phase, it is best to set it to the same value as restarts.increase_npt_amt. Default is 1.
- restarts.hard.use_old_rk If using hard restarts, whether or not to recycle the objective value at the best iterate found when performing a restart. This saves one objective evaluation. Default is True.
- restarts.max_npt Maximum allowed value of $|Y_k|$, useful if increasing with each restart. Default is npt, the input parameter to dfols.solve().
- restarts.soft.max_fake_successful_steps The maximum number of successful steps in a given run where the new (smaller) objective value is larger than the best value found in a previous run. Default is maxfun, the input to dfols.solve().
- restarts.auto_detect Whether or not to automatically determine when to restart. This is an extra condition, and restarts can still be triggered by small trust region radius, etc. Default is True.
- restarts.auto_detect.history How many iterations of data on model changes and trust region radii to store. There are two criteria used: trust region radius decreases (no increases over the history, more decreases than no changes), and change in model Jacobian (consistently increasing trend as measured by slope and correlation coefficient of line of best fit). Default is 30.
- restarts.auto_detect.min_chgJ_slope Minimum rate of increase of $\log(\|J_k J_{k-1}\|_F)$ over the past iterations to cause a restart. Default is 0.015.
- restarts.auto_detect.min_correl Minimum correlation of the data set $(k, \log(\|J_k J_{k-1}\|_F))$ required to cause a restart. Default is 0.1.

4.11 Dynamically Growing Initial Set

- growing.ndirs_initial Number of initial points to add (excluding x_k). This should only be changed to a value less than n, and only if the default setup cost of n+1 evaluations of objfun is impractical. If this is set to be less than the default, the input value npt should be set to n. If the default is used, all the below parameters have no effect on DFO-LS. Default is npt-1.
- growing.full_rank.use_full_rank_interp If growing.ndirs_initial is less than npt, whether to perturb the interpolated J_k to make it full rank, allowing the trust region step to include components in the full search space. Default is True if $m \geq n$ and False otherwise (opposite to growing. perturb_trust_region_step).
- growing.perturb_trust_region_step Whether to perturb the trust region step by an orthogonal direction not yet searched. This is an alternative to growing.full_rank.use_full_rank_interp. Default is False if $m \geq n$ and True otherwise (opposite to growing.full_rank.use_full_rank_interp).
- growing.delta_scale_new_dirns When adding new search directions, the length of the step as a multiple of Δ_k . Default is 1, or 0.1 if growing.perturb_trust_region_step=True.
- growing.full_rank.scale_factor Magnitude of extra components added to J_k . Default is 10^{-2} .
- growing.full_rank.svd_scale_factor-Floor singular values of J_k at this factor of the last nonzero value. Default is 1.
- growing.full_rank.min_sing_val Absolute floor on singular values of J_k . Default is 10^{-6} .
- growing.full_rank.svd_max_jac_cond Cap on condition number of J_k after applying floors to singular values (effectively another floor on the smallest singular value, since the largest singular value is fixed). Default is 10^8 .

- growing.do_geom_steps While still growing the initial set, whether to do geometry-improving steps in the trust region algorithm, as per the usual algorithm. Default is False.
- growing.safety.do_safety_step While still growing the initial set, whether to perform safety steps, or the regular trust region steps. Default is True.
- growing.safety.reduce_delta While still growing the initial set, whether to reduce Δ_k in safety steps. Default is False.
- growing.safety.full_geom_step While still growing the initial set, whether to do a full geometry-improving step within safety steps (the same as the post-growing phase of the algorithm). Since this involves reducing Δ_k , cannot be True if growing.safety.reduce_delta is True. Default is False.
- growing.reset_delta Whether or not to reset trust region radius Δ_k to its initial value at the end of the growing phase. Default is False.
- growing.reset_rho Whether or not to reset trust region radius lower bound ρ_k to its initial value at the end of the growing phase. Default is False.
- growing.gamma_dec Trust region decrease parameter during the growing phase. Default is tr_radius.gamma_dec.
- growing.num_new_dirns_each_iter Number of new search directions to add with each iteration where we do not have a full set of search directions. Default is 0, as this approach is not recommended.

4.12 Dykstra's Algorithm

- dykstra.d_tol Tolerance on the stopping conditions of Dykstra's algorithm. Default is 10^{-10} .
- dykstra.max_iters The maximum number of iterations Dykstra's algorithm is allowed to take before stopping. Default is 100.

4.13 Checking Matrix Rank

• matrix_rank.r_tol - Tolerance on what is the smallest possible diagonal entry value in the QR factorization before being considered zero. Default is 10^{-18} .

4.14 References

DIAGNOSTIC INFORMATION

In *Using DFO-LS*, we saw that the output of DFO-LS returns a container which includes diagnostic information about the progress of the algorithm (soln.diagnostic_info). This object is a Pandas DataFrame, with one row per iteration of the algorithm. In this section, we explain the meaning of each type of output (the columns of the DataFrame).

To save this information to a CSV file, use:

```
# Previously: define objfun and x0

# Turn on diagnostic information
user_params = {'logging.save_diagnostic_info': True}

# Call DFO-LS
soln = dfols.solve(objfun, x0, user_params=user_params)

# Save diagnostic info to CSV
soln.diagnostic_info.to_csv('myfile.csv')
```

Depending on exactly how DFO-LS terminates, the last row of results may not be fully populated.

5.1 Current Iterate

- xk Best point found so far (current iterate). This is only saved if user_params['logging.save_xk'] = True.
- rk The vector of residuals at the current iterate. This is only saved if user_params['logging. save_rk'] = True.
- fk The value of f at the current iterate.

5.2 Trust Region

- rho The lower bound on the trust region radius ρ_k .
- delta The trust region radius Δ_k .
- norm_sk The norm of the trust region step $||s_k||$.

5.3 Model Interpolation

- npt The number of interpolation points.
- interpolation_error The sum of squares of the interpolation errors from the interpolated model.
- interpolation_condition_number The condition number of the matrix in the interpolation linear system.
- interpolation_change_J_norm The Frobenius norm of the change in Jacobian at this iteration, $||J_k J_{k-1}||_F$.
- interpolation_total_residual The total residual from the interpolation optimization problem.
- poisedness The smallest value of Λ for which the current interpolation set Y_k is Λ -poised in the current trust region. This is the most expensive piece of information to compute, and is only computed if user_params['logging.save_poisedness' = True.
- max_distance_xk The maximum distance from any interpolation point to the current iterate.
- norm_gk The norm of the model gradient $||g_k||$.

5.4 Iteration Count

- nruns The number of times the algorithm has been restarted.
- nf The number of objective evaluations so far (see soln.nf)
- nx The number of points at which the objective has been evaluated so far (see soln.nx)
- nsamples The total number of objective evaluations used for all current interpolation points.
- iter_this_run The number of iterations since the last restart.
- iters_total The total number of iterations so far.

5.5 Algorithm Progress

- iter_type A text description of what type of iteration we had (e.g. Successful, Safety, etc.)
- ratio The ratio of actual to predicted objective reduction in the trust region step.
- slow_iter Equal to 1 if the current iteration is successful but slow, 0 if is successful but not slow, and -1 if
 was not successful.

VERSION HISTORY

This section lists the different versions of DFO-LS and the updates between them.

6.1 Version 1.0 (6 Feb 2018)

· Initial release of DFO-LS

6.2 Version 1.0.1 (20 Feb 2018)

• Minor bug fix to trust region subproblem solver (the output crymin is calculated correctly) - this has minimal impact on the performance of DFO-LS.

6.3 Version 1.0.2 (20 Jun 2018)

- Extra optional input args which passes through arguments for objfun.
- Bug fixes: default parameters for reduced initialization cost regime, returning correct value if exiting from within a safety step, retrieving dependencies during installation.

6.4 Version 1.1 (16 Jan 2019)

- Use different default reduced initialization cost method for inverse problems to ensure whole space is searched correctly.
- Bug fixes: default trust region radius when scaling feasible region, exit correctly when no Jacobian returned, handling overflow at initial value

6.5 Version 1.1.1 (5 Apr 2019)

• Link code to Zenodo, to create DOI - no changes to the DFO-LS algorithm.

6.6 Version 1.2 (12 Feb 2020)

- Use deterministic initialisation by default (so it is no longer necessary to set a random seed for reproducibility of DFO-LS results).
- Full model Hessian stored rather than just upper triangular part this improves the runtime of Hessian-based operations.
- Faster trust-region and geometry subproblem solutions in Fortran using the trustregion package.
- Faster interpolation solution for multiple right-hand sides.
- Don't adjust starting point if it is close to the bounds (as long as it is feasible).
- Option to stop default logging behavior and/or enable per-iteration printing.
- · Bugfix: correctly handle 1-sided bounds as inputs, avoid divide-by-zero warnings when auto-detecting restarts.

6.7 Version 1.2.1 (13 Feb 2020)

• Make the use of the trustregion package optional, not installed by default.

6.8 Version 1.2.2 (26 Feb 2021)

Minor update to remove NumPy deprecation warnings - no changes to the DFO-LS algorithm.

6.9 Version 1.2.3 (1 Jun 2021)

Minor update to customise handling of NaNs in objective evaluations - no changes to the DFO-LS algorithm.

6.10 Version 1.3.0 (8 Nov 2021)

- Handle finitely many arbitrary convex constraints in addition to simple bound constraints.
- Add module-level logging for more informative log outputs.
- Only new functionality is added, so there is no change to the solver for unconstrained/bound-constrained problems.

CHAPTER

SEVEN

CONTRIBUTORS

7.1 Main author

• Lindon Roberts (Australian National University)

7.2 Contributors

• Matthew Hough (University of Waterloo): handle general convex constraints [version 1.3]

CHAPTER

EIGHT

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