
pyOptSparse

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Aug 18, 2022

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pyOptSparse is an object-oriented framework for formulating and solving nonlinear constrained optimization problems in an efficient, reusable, and portable manner. Some key features of pyOptSparse include:

- Object-oriented development, which maintains independence between the optimization problem formulation and its solution by different optimizers
- The use of sparse matrices throughout the code, to more efficiently handle large-scale optimization problems
- Parallel model execution under MPI, both for expensive analyses that must be done in parallel, and for parallel function evaluation when using certain gradient-free optimizers
- The optimization histories can be stored during the optimization process, and a partial history can also be used to hot-restart the optimization
- A post-processing GUI utility called OptView to analyze optimization results

pyOptSparse is a fork of [pyOpt](#). However, it is not backwards compatible with pyOpt and thus optimization scripts will need to be modified to use pyOptSparse.

GETTING STARTED

To get started, please see the *Installation Instructions* and the *Quickstart*.

1.1 Installation Instructions

1.1.1 Conda

Conda packages are available on `conda-forge` and can be installed via

```
$ conda install -c conda-forge pyoptsparse
```

This would install `pyOptSparse` with the built-in optimizers, as well as `IPOPT`. If you wish to use optimizers not packaged by conda, e.g. `SNOPT`, then you must build the package from source.

1.1.2 Building from source

Requirements

`pyOptSparse` has the following dependencies:

- Python 3.7 or 3.8, though other Python 3 versions will likely work
- C and Fortran compilers. We recommend `gcc` and `gfortran` which can be installed via the package manager for your operating system.

Please make sure these are installed and available for use. In order to use `NSGA2`, `SWIG` (v1.3+) is also required, which can be installed via the package manager. If those optimizers are not needed, then you do not need to install `SWIG`. Simply comment out the corresponding lines in `pyoptsparse/pyoptsparse/setup.py` so that they are not compiled. The corresponding lines in `pyoptsparse/pyoptsparse/__init__.py` must be commented out as well.

Python dependencies are automatically handled by `pip`, so they do not need to be installed separately. The only exception is `numpy`, which is required as part of the build process and therefore must be present before installing.

Note:

- In Linux, the python header files (`python-dev`) are also required.
 - **We do not support operating systems other than Linux.** For macOS users, the conda package may work out of the box if you do not need any non-default optimizers. For Windows users, a conda package is on the way, if it's not already in the repos. This comes with the same disclaimer as the macOS conda package. Alternatively, follow the *conda build instructions* below as this will work on any platform.
-

Installation

The easiest and recommended way to install pyOptSparse is with `pip`. First clone the repository into a location which is not on the `$PYTHONPATH`, for example `$HOME/packages/`. Then in the root `pyoptsparse` folder type

```
$ pip install .
```

For those not using virtual environments, a user install may be needed

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

If you plan to modify pyOptSparse, installing with the developer option, i.e. with `-e`, will save you from re-installing each time you modify the Python code.

Note: Some optimizers are proprietary, and their sources are not distributed with pyOptSparse. To use them, please follow the instructions on specific optimizer pages.

Specifying compilers

To specify a non-default compiler (e.g. something other than `/usr/bin/gcc`), meson recognizes certain [special environment variables](#). For example, to specify the Intel compilers, simply run

```
$ FC=$(which ifort) CC=$(which icc) pip install .
```

1.1.3 Installing OptView

OptView and OptView-Dash have separate dependencies that must be installed. To install pyOptSparse including those dependencies, run

```
$ pip install .[optview]
```

1.1.4 Testing

pyOptSparse provides a set of unit and regression tests to verify the installation. To run these tests, first install `testflo` which is a testing framework developed by the OpenMDAO team:

```
$ pip install testflo
```

Then, in the project root directory, type:

```
$ testflo . -v
```

to run all tests.

1.1.5 Update or Uninstall

To update pyOptSparse, first delete the `meson_build` directory, then update the package using `git`. For stability, users are encouraged to stick to tagged releases. Install the package normally via `pip`.

To uninstall the package, type

```
$ pip uninstall pyoptsparse
```

1.1.6 Conda Build Instructions

The following instructions explain how to build and install pyOptSparse in a conda environment. This has the advantage that conda can be used to install all the necessary dependencies in an isolated and reproducible environment. Considering how finicky Windows can be with ABI compatibility among various compilers, this is the recommended approach. The guide will work on any platform, however.

The only build requirement for the build is a working conda installation as all compilers and dependencies are pulled from the conda-forge repos, with the exception of a Windows build, which requires Visual Studio 2017 C++ Build Tools.

First, we need to create the conda environment. An `environment.yml` file is provided in the pyoptsparse repo:

Linux/OSX

Windows

```
conda create -y -n pyos-build
conda activate pyos-build
conda config --env --add channels conda-forge
conda config --env --set channel_priority strict

conda env update -f .github/environment.yml
```

```
conda create -y -n pyos-build
conda activate pyos-build
conda config --env --add channels conda-forge
conda config --env --set channel_priority strict

conda env update -f .github\environment.yml
conda install libpgmath
```

Next, we need to tell the compiler where to find IPOPT:

Linux/OSX

Windows

```
export IPOPT_DIR="$CONDA_PREFIX"
```

```
set IPOPT_DIR=%CONDA_PREFIX%\Library
```

Finally, build the wheel and install it using pip:

Linux/OSX

Windows

```
# build wheel
python -m build -n -x .

# install wheel
pip install --no-deps --no-index --find-links dist pyoptsparse
```

```
# set specific compiler flags
set CC=cl
set FC=flang
```

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```
set CC_LD=link

# build wheel
python -m build -n -x .

# install wheel
pip install --no-deps --no-index --find-links dist pyoptsparse
```

1.2 Quickstart

The following shows how to get started with pyOptSparse by solving Schittkowski's TP37 constrained problem. First, we show the complete program listing and then go through each statement line by line:

```
# First party modules
from pyoptsparse import SLSQP, Optimization

# rst begin objfunc
def objfunc(xdict):
    x = xdict["xvars"]
    funcs = {}
    funcs["obj"] = -x[0] * x[1] * x[2]
    conval = [0] * 2
    conval[0] = x[0] + 2.0 * x[1] + 2.0 * x[2] - 72.0
    conval[1] = -x[0] - 2.0 * x[1] - 2.0 * x[2]
    funcs["con"] = conval
    fail = False

    return funcs, fail

# rst begin optProb
# Optimization Object
optProb = Optimization("TP037 Constraint Problem", objfunc)

# rst begin addVar
# Design Variables
optProb.addVarGroup("xvars", 3, "c", lower=[0, 0, 0], upper=[42, 42, 42], value=10)

# rst begin addCon
# Constraints
optProb.addConGroup("con", 2, lower=None, upper=0.0)

# rst begin addObj
# Objective
optProb.addObj("obj")

# rst begin print
# Check optimization problem
print(optProb)
```

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```

# rst begin OPT
# Optimizer
optOptions = {"IPRINT": -1}
opt = SLSQP(options=optOptions)

# rst begin solve
# Solve
sol = opt(optProb, sens="FD")

# rst begin check
# Check Solution
print(sol)

```

Start by importing the pyOptSparse package:

```

# First party modules
from pyoptsparse import SLSQP, Optimization

```

Next we define the objective function that takes in the design variable *dictionary* and returns a *dictionary* containing the constraints and objective, as well as a (boolean) flag indicating if the objective function evaluation was successful. For the TP37, the objective function is a simple analytic function:

```

def objfunc(xdict):
    x = xdict["xvars"]
    funcs = {}
    funcs["obj"] = -x[0] * x[1] * x[2]
    conval = [0] * 2
    conval[0] = x[0] + 2.0 * x[1] + 2.0 * x[2] - 72.0
    conval[1] = -x[0] - 2.0 * x[1] - 2.0 * x[2]
    funcs["con"] = conval
    fail = False

    return funcs, fail

```

Notes:

- The `xdict` variable is a dictionary whose keys are the names from each `addVar` and `addVarGroup` call. The line

```
x = xdict["xvars"]
```

retrieves an array of length 3 which are all the variables for this optimization.

- The line

```
conval = [0] * 2
```

creates a list of length 2, which stores the numerical values of the two constraints. The `funcs` dictionary return must contain keys that match the constraint names from `addCon` and `addConGroup` as well as the objectives from `addObj` calls. This is done in the following calls:

```
funcs["obj"] = -x[0] * x[1] * x[2]
funcs["con"] = conval
```

Now the optimization problem can be initialized:

```
# Optimization Object
optProb = Optimization("TP037 Constraint Problem", objfunc)
```

This creates an instance of the optimization class with a name and a reference to the objective function. To complete the setup of the optimization problem, the design variables and constraints need to be defined.

Design variables and constraints can be added either one-by-one or as a group. Adding variables by group is generally recommended for related variables:

```
# Design Variables
optProb.addVarGroup("xvars", 3, "c", lower=[0, 0, 0], upper=[42, 42, 42], value=10)
```

This call adds a group of 3 variables with name `xvars`. The variable bounds (side constraints) are 0 for the lower bounds, and 42 for the upper bounds. The initial values for each variable is 10.0.

Now, we must add the constraints. Like design variables, these may be added individually or by group. It is recommended that related constraints are added by group where possible:

```
# Constraints
optProb.addConGroup("con", 2, lower=None, upper=0.0)
```

This call adds two variables with name `con`. There is no lower bound for the variables and the upper bound is 0.0.

We must also assign the the key value for the objective using the `addObj` call:

```
# Objective
optProb.addObj("obj")
```

The optimization problem can be printed to verify that it is set up correctly:

```
# Check optimization problem
print(optProb)
```

which produces the following table:

```
Optimization Problem -- TP037 Constraint Problem
=====
Objective Function: objfunc

Objectives
  Index  Name      Value
    0    obj      0.000000E+00

Variables (c - continuous, i - integer, d - discrete)
```

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Index	Name	Type	Lower Bound	Value	Upper Bound	Status
0	xvars_0	c	0.000000E+00	1.000000E+01	4.200000E+01	
1	xvars_1	c	0.000000E+00	1.000000E+01	4.200000E+01	
2	xvars_2	c	0.000000E+00	1.000000E+01	4.200000E+01	

Constraints (i - inequality, e - equality)						
Index	Name	Type	Lower	Value	Upper	Status
↪ Lagrange Multiplier (N/A)						
0	con	i	-1.000000E+20	0.000000E+00	0.000000E+00	u 9.
↪ 000000E+100						
1	con	i	-1.000000E+20	0.000000E+00	0.000000E+00	u 9.
↪ 000000E+100						

To solve an optimization problem with pyOptSparse an optimizer must be initialized. The initialization of one or more optimizers is independent of the initialization of the optimization problem. To initialize SLSQP, which is an open-source, sequential least squares programming algorithm that comes as part of the pyOptSparse package, use:

```
# Optimizer
optOptions = {"IPRINT": -1}
opt = SLSQP(options=optOptions)
```

This initializes an instance of SLSQP with the option IPRINT set to -1. All other options will be set to the default values, which can be found on the optimizer-specific pages. For example, the default options for SLSQP can be found in the page [SLSQP](#).

Now TP37 can be solved using pyOptSparse's automatic finite difference for the gradients:

```
# Solve
sol = opt(optProb, sens="FD")
```

We can print the solution objection to view the result of the optimization:

```
# Check Solution
print(sol)
```

which produces the following output:

```
Optimization Problem -- TP037 Constraint Problem
```

```
=====
Objective Function: objfunc
```

```
Solution:
```

```
-----
Total Time:                0.0062
  User Objective Time :    0.0001
  User Sensitivity Time :  0.0011
  Interface Time :        0.0046
  Opt Solver Time:        0.0003
Calls to Objective Function :    22
Calls to Sens Function :        8
```

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Objectives							
Index	Name	Value					
0	obj	-3.456000E+03					
Variables (c - continuous, i - integer, d - discrete)							
Index	Name	Type	Lower Bound	Value	Upper Bound	Status	
0	xvars_0	c	0.000000E+00	2.399997E+01	4.200000E+01		
1	xvars_1	c	0.000000E+00	1.200001E+01	4.200000E+01		
2	xvars_2	c	0.000000E+00	1.200000E+01	4.200000E+01		
Constraints (i - inequality, e - equality)							
Index	Name	Type	Lower	Value	Upper	Status	
↔Lagrange Multiplier (N/A)							
0	con	i	-1.000000E+20	7.564591E-07	0.000000E+00	u	9.
↔000000E+100							
1	con	i	-1.000000E+20	-7.200000E+01	0.000000E+00		9.
↔000000E+100							

1.3 Guide

pyOptSparse is designed to solve general, constrained nonlinear optimization problems of the form:

$$\begin{aligned} & \min f(x) \\ & \text{with respect to } x \\ & \text{such that } g_{j,L} \leq g_j(x) \leq g_{j,U}, \quad j = 1, \dots, m \\ & \quad \quad \quad x_{i,L} \leq x_i \leq x_{i,U}, \quad i = 1, \dots, n \end{aligned}$$

where: x is the vector of n design variables, $f(x)$ is a nonlinear function, and $g(x)$ is a set of m nonlinear functions.

Equality constraints are specified using the same upper and lower bounds for the constraint. i.e., $g_{j,L} = g_{j,U}$. The ordering of the constraints is arbitrary; pyOptSparse reorders the problem automatically depending on the requirements of each individual optimizer.

The optimization class is created using the following call:

```
optProb = Optimization("name", objFun)
```

The general template of the objective function is as follows:

```
def obj_fun(xdict):
    funcs = {}
    funcs["obj_name"] = function(xdict)
    funcs["con_name"] = function(xdict)
    fail = False # Or True if an analysis failed

    return funcs, fail
```

where:

- `funcs` is the dictionary of constraints and objective value(s)

- `fail` can be a Boolean or an int. False (or 0) for successful evaluation and True (or 1) for unsuccessful. Can also be 2 when using SNOPT and requesting a clean termination of the run.

If the Optimization problem is unconstrained, `funcs` will contain only the objective key(s).

1.3.1 Design Variables

The simplest way to add a single continuous variable with no bounds (side constraints) and initial value of 0.0 is to simply call `addVar`:

```
optProb.addVar("var_name")
```

This will result in a scalar variable included in the `x` dictionary call to `obj_fun` which can be accessed by doing

```
x["var_name"]
```

A more complex example will include lower bounds, upper bounds and a non-zero initial value:

```
optProb.addVar("var_name", lower=-10, upper=5, value=-2)
```

The `lower` or `upper` keywords may be specified as `None` to signify there is no bound on the variable.

Finally, an additional keyword argument `scale` can be specified which will perform an internal design variable scaling. The `scale` keyword will result in the following:

$$x_{\text{opt}} = x_{\text{user}} \times \text{scale}$$

The purpose of the scale factor is ensure that design variables of widely different magnitudes can be used in the same optimization. It is desirable to have the magnitude of all variables within an order of magnitude or two of each other.

The `addVarGroup` call is similar to `addVar` except that it adds a group of 1 or more variables. These variables are then returned as a numpy array within the `x`-dictionary. For example, to add 10 variables with no lower bound, and a scale factor of 0.1:

```
optProb.addVarGroup("con_group", 10, upper=2.5, scale=0.1)
```

1.3.2 Constraints

The simplest way to add a single constraint with no bounds (i.e., not a very useful constraint!) is to use the function `addCon`:

```
optProb.addCon("not_a_real_constraint")
```

To include bounds on the constraints, use the `lower` and `upper` keyword arguments. If `lower` and `upper` are the same, it will be treated as an equality constraint:

```
optProb.addCon("inequality_constraint", upper=10)
optProb.addCon("equality_constraint", lower=5, upper=5)
```

Like design variables, it is often necessary to scale constraints such that all constraint values are approximately the same order of magnitude. This can be specified using the `scale` keyword:

```
optProb.addCon("scaled_constraint", upper=10000, scale=1.0 / 10000)
```

Even if the `scale` keyword is given, the `lower` and `upper` bounds are given in their un-scaled form. Internally, `pyOptSparse` will use the scaling factor to produce the following constraint:

$$\text{con}_{\text{opt}} = \text{con}_{\text{user}} \times \text{scale}$$

In the example above, the constraint values are divided by 10000, which results in a upper bound (that the optimizer sees) of 1.0.

Constraints may also be flagged as linear using the `linear=True` keyword option. Some optimizers can perform special treatment on linear constraint, often ensuring that they are always satisfied exactly on every function call (SNOPT for example). Linear constraints also require the use of the `wrt` and `jac` keyword arguments. These are explained below.

One of the major goals of `pyOptSparse` is to enable the use of sparse constraint Jacobians, hence the *Sparse* in the name! Manually computing sparsity structure of the constraint Jacobian is tedious at best and become even more complicated as optimization scripts are modified by adding or deleting design variables and/or constraints. `pyOptSparse` is designed to greatly facilitate the assembly of sparse constraint Jacobians, alleviating the user of this burden. The idea is that instead of the user computing a dense matrix representing the constraint Jacobian, a “dictionary of keys” approach is used which allows incrementally specifying parts of the constraint Jacobian. Consider the optimization problem given below:

	varA (3)	varB (1)	varC (3)
conA (2)		X	X
conB (2)	X		X
conC (4)	X	X	X
conD (3)			X

The X’s denote which parts of the Jacobian have non-zero values. `pyOptSparse` does not determine the sparsity structure of the Jacobian automatically, it must be specified by the user during calls to `addCon` and `addConGroup`. By way of example, the code that generates the hypothetical optimization problem is as follows:

```
optProb.addVarGroup("varA", 3)
optProb.addVarGroup("varB", 1)
optProb.addVarGroup("varC", 3)

optProb.addConGroup("conA", 2, upper=0.0, wrt=["varB", "varC"])
optProb.addConGroup("conB", 2, upper=0.0, wrt=["varC", "varA"])
optProb.addConGroup("conC", 4, upper=0.0)
optProb.addConGroup("conD", 3, upper=0.0, wrt=["varC"])
```

Note that the order of the `wrt` (which stands for with-respect-to) is not significant. Furthermore, if the `wrt` argument is omitted altogether, `pyOptSparse` assumes that the constraint is dense.

To examine the sparsity pattern, `pyOptSparse` can generate the ASCII table shown above. To do so, use the following call after adding all the design variables, objectives and constraints:

```
optProb.printSparsity()
```

Using the `wrt` keyword allows the user to determine the overall sparsity structure of the constraint Jacobian. However, we have currently assumed that each of the blocks with an X in is a dense sub-block. `pyOptSparse` allows each of the *sub-blocks* to itself be sparse. `pyOptSparse` requires this sparsity structure to be specified when the constraint is added. This information is supplied through the `jac` keyword argument. Lets say, that the (conD, varC) block of the Jacobian is actually a sparse and linear. By way of example, the call instead may be as follows:

```

jac = sparse.lil_matrix((3, 3))
jac[0, 0] = 1.0
jac[1, 1] = 4.0
jac[2, 2] = 5.0

optProb.addConGroup("conD", 3, upper=0.0, wrt=["varC"], linear=True, jac={"varC": jac})

```

We have created a linked list sparse matrix using `scipy.sparse`. Any SciPy sparse matrix format can be accepted. We have then provided this constraint Jacobian using the `jac` keyword argument. This argument is a dictionary, and the keys must match the design variable sets given in the `wrt` to keyword. Essentially what we have done is specified the which blocks of the constraint rows are non-zero, and provided the sparsity structure of ones that are sparse.

For linear constraints the values in `jac` are meaningful: they must be the actual linear constraint Jacobian values (which do not change). For non-linear constraints, only the sparsity structure (i.e. which entries are nonzero) is significant. The values themselves will be determined by a call to the `sens()` function.

Also note, that the `wrt` and `jac` keyword arguments are only supported when user-supplied sensitivity is used. If automatic gradients from pyOptSparse are used, the constraint Jacobian will necessarily be dense.

Note: Currently, only the optimizers SNOPT and IPOPT support sparse Jacobians.

1.3.3 Objectives

Each optimization will require at least one objective to be added. This is accomplished using a the call to `addObj`:

```
optProb.addObj("obj_name")
```

What this does is tell pyOptSparse that the key `obj_name` in the function returns will be taken as the objective. For optimizers that can do multi-objective optimization (e.g. NSGA2), multiple objectives can be added. Optimizers that can only handle one objective enforce that only a single objective is added to the optimization description.

1.3.4 Specifying Derivatives

Approximating Derivatives

pyOptSparse can automatically compute derivatives of the objective and constraint functions using finite differences or the complex-step method. This is done by simply passing a string to the `sens=` argument when calling an optimizer. See the possible values [here](#). In the simplest case, using `sens="FD"` will be enough to run an optimization using forward differences with a default step size.

Analytic Derivatives

If analytic derivatives are available, users can compute them within a user-defined function. This function accepts as inputs a dictionary containing design variable values as well as another dictionary containing objective and constraint values. It returns a nested dictionary containing the gradients of the objective and constraint values with respect to those design variables at the current design point. Specifically, the first-layer keys should be associated with objective and constraint names while the second-layer keys correspond to design variables. The dictionary values are the computed analytic derivatives, either in the form of lists or NumPy arrays with the expected shape. Since pyOptSparse uses string indexing, users need to make sure the keys in the returned dictionary are consistent with the names of design variables, constraints and objectives which were first added to the optimization problem.

Tip:

1. Only the non-zero sub-blocks of the Jacobian need to be defined in the dictionary, and pyOptSparse will assume the rest to be zero.
 2. Derivatives of the linear constraints do not need to be given here, since they are constant and should have already been specified via the `jac=` keyword argument when adding the constraint.
-

For example, if the optimization problem has one objective `obj`, two constraints `con`, and three design variables `xvars`, the returned sensitivity dictionary (with placeholder values) should have the following structure:

```
{"obj": {"xvars": [1, 2, 3]}, "con": {"xvars": [[4, 5, 6], [7, 8, 9]]}}
```

Once this function is constructed, users can pass its function handle to the optimizer when it's called via:

```
sol = opt(optProb, sens=sens, ...)
```

1.3.5 Optimizer Instantiation

There are two ways to instantiate the optimizer object. The first, and most explicit approach is to directly import the optimizer class, for example via

```
from pyoptsparse import SLSQP  
  
opt = SLSQP(...)
```

However, in order to easily switch between different optimizers without having to import each class, a convenience function called `OPT` is provided. It accepts a string argument in addition to the usual options, and instantiates the optimizer object based on the string:

```
from pyoptsparse import OPT  
  
opt = OPT("SLSQP", ...)
```

Note that the name of the optimizer is case-insensitive, so `slsqp` can also be used. This makes it easy to for example choose the optimizer from the command-line, or more generally select the optimizer using strings without preemptively importing all classes.

1.4 Advanced Features

1.4.1 MPI handling

pyOptSparse can optionally run in parallel if a suitable `mpi4py` installation exists. This will be automatically detected and imported at run-time.

If you only want to run in parallel, you can force pyOptSparse to do so by setting the environment variable `PYOPTSPARSE_REQUIRE_MPI` to any one of these values: `['always', '1', 'true', 'yes']` If a suitable `mpi4py` is not available, an exception will be raised and the run terminated.

If you explicitly do not wish to use `mpi4py`, set the environment variable `PYOPTSPARSE_REQUIRE_MPI` to anything other than those values. This can come in handy, for example, if your MPI installation is not functioning properly, but you still need to run serial code.

1.4.2 Storing Optimization History

pyOptSparse includes a *History* class that stores all the relevant optimization information in an SQL database. This database is updated at every optimization iteration, and can be accessed via both the API described in the linked section, and via *OptView*. By default, the history file is NOT written. To turn the history recording on, use the `storeHistory` attribute when invoking the optimization run, e.g.:

```
sol = opt(optProb, sens=sens, storeHistory="<your-history-file-name>.hst", ...)
```

1.4.3 Hot start

Hot start refers to the way optimizations are initialized. Such start-up procedure is named in contrast to the regular optimization initialization, or “cold start”, in which case pyOptSparse simply initializes an optimization job from scratch, using initial design variables set by the user. There are several situations in which such cold starts can be avoided by leveraging on the information from a previous optimization, with the aim to reduce the overall computational time. Suppose you run an optimization that was accidentally terminated prematurely by, for example, an excessively-low iteration limit. If you restarted the optimization using the DVs from the last iteration (but losing all the accumulated history), you will start from a better initial point but will likely incur in a performance penalty. The overall optimization, now split between two jobs, will end up taking far more steps than it would’ve taken if the original optimization was allowed to progress. This is due to the fact that some of the optimizers wrapped in pyOptSparse need a few initial iterations to build a (local) approximation of the design space. Because of this lack of information, there is a start-up cost to a cold started optimization, where the optimizer has to spend time rebuilding the information. In a sense, for many optimizers the next iterate does not depend only on the current iterate, but effectively all the previous iterates as well!

Hot starting optimizations is a way to address this issue. pyOptSparse has the ability to read in the previous optimization history file, and *replay* the entire history starting at the original design variables, feeding `funcs` to the optimizer each time. For a deterministic optimizer, if all solver settings remain the same, then it should request the same sequence of iterates (up to machine precision), and if those have been previously evaluated, they are read from the history file and passed to the optimizer. If at any point the requested design variables diverge from the history, then we will actually perform a function evaluation, and all subsequent points will be newly evaluated. For this process to work, the following must be true:

- The optimizer is deterministic. Note that a stochastic optimizer can still be made deterministic even if it uses random numbers, as long as the random seed is fixed. If the optimizer performs a random gradient check (e.g. SNOPT), it’s best to disable these just in case.
- Optimizer settings that affect the path of the optimization must remain the same. It is perfectly fine to change for example settings related to print outs, but not those affecting the line search.

To use the hot start feature, simply call the optimizer with the option `hotStart = <hot start file>`. See the API documentation for each optimizer for more information. Because the hot start process will store all the previous “restarted” iterations in the new history file, it’s possible to restart as many times as you like, each time using the previous history file.

1.4.4 Time limit (for SNOPT only)

The *Optimizer* class in pyOptSparse has an attribute used to set the maximum allowable wall time for optimizations using SNOPT. The code will exit gracefully when such time limit is reached. This feature is particularly useful when running a time-constrained job, as in the case of most HPC systems. To enable this feature, use the `timeLimit` option when invoking the optimizer, as shown below:

```
sol = opt(optProb, sens=sens, timeLimit=24 * 3600, ...)
```

Note that the attribute takes the maximum wall time *in seconds* as an integer number.

Note: pyOptSparse will verify that the computational time is not exceeded before proceeding to the next iteration. It will NOT interrupt an ongoing function or sensitivity evaluation. If your function evaluations are expensive, you should be more conservative when setting the `timeLimit` option for it to be effective.

1.5 Post-processing

There are three post-processing utilities that are provided with pyOptSparse.

- OptView is a GUI designed to quickly and interactively visualize optimization histories
- OptView-Dash is a [Dash](#) implementation of OptView
- History is a Python class that can be used to read in the history file, and provide API for programmatically extracting data.

1.5.1 OptView

Requirements

OptView has the following dependency tree:

```
matplotlib (OptView)
  \-backends
    | \-backend_tkagg
    |   \-FigureCanvasTkAgg (OptView)
    |     \-NavigationToolbar2TkAgg (OptView)
    \-pyplot (OptView)
mpl_toolkits
  \-axes_grid1
  | \-host_subplot (OptView)
  \-axisartist (OptView)
numpy (OptView)
```

For installation instructions, see [Installing OptView](#). Although not necessary for most usage, the `dill` package is needed if you wish to save an editable version of the graph produced in OptView. `dill` can be installed via `pip` in a terminal using

```
$ pip install dill
```

`view_saved_figure.py` can be used to reformat and view the saved figure.

Usage

OptView can be run via terminal from any directory as

```
$ optview histFile
```

Here, `histFile` is the name of the history file to be examined (default is `opt_hist.hst`).

Additionally, you can open multiple history files in the same OptView instance by calling them via the command line

```
$ optview histFile1 histFile2 histFile3
```

Each file's contents will be loaded into OptView with a flag appended to the end of each variable or function name corresponding to the history file. The first one listed will have `'_A'` added to the name, the second will have `'_B'` added, etc. There is currently no limit to the number of history files than can be loaded.

Optionally, if you want to save the generated figures, there is an optional argument:

```
$ optview histFile --output ~/my_figures
```

`outputDirectory` is the name of the desired output directory for saved images. By default, the figure is saved to the directory where you invoked `optview`.

Features

OptView has many options and features, including:

- plotting multiple variables on a single plot
- producing stacked plots
- live searchable variable names
- hovering plot labels
- saving the figure to an image or pickling it for later formatting
- refreshing the optimization history on the fly

Although some of these are self-explanatory, the layout and usage of OptView will be explained below.

GUI Layout

The window is divided into two sections. The top is the canvas where the figure and graphs will be produced, while the bottom grayed section contains user-selectable options. Here, we will focus on the user options.

The selectable variables are contained on the left hand side of the options panel in scrollable listboxes. You can select multiple items from the listboxes using the normal selection operators such as control and shift. If a selected variable is an array, a third listbox should appear on the right hand side of the options panel, allowing you to select specific sub-variables within the single array variable.

There are three main options when selecting how to produce the graph(s):

- Shared axes - all selected variables are plotted on a single pair of axes
- Multiple axes - each selected variable gets its own y-axis while all selected data shares an x-axis
- Stacked plots - each variable gets its own individual plot and the set is stacked vertically

Most checkbox options should play well with any of these three main options, though there are known issues with using the 'multiple axes' option and delta values or for displaying arrays.

There are seven checkbox options:

- Absolute delta values - displays the absolute difference between one iteration's value and the previous
- Log scale - sets the y-axis as a log scale
- Min/max for arrays - only shows the minimum and maximum value of a variable for each iteration
- Show all for arrays - plots all variables within an array
- Show legend - reveals the legend for the plotted data
- Show bounds - shows the variable bounds as dashed lines
- Show 'major' iterations - a filter to remove the line search iterations from the plotting results; especially useful for SNOPT output

Additionally, four buttons allow control of the plot:

- Refresh history - reloads the history file; used if checking on an optimization run on the fly
- Save all figures - saves .png versions of a basic plot for each variable in the history file
- Save figure - saves a .png and .pickle version of the current plot (the .pickle version can be reformatted afterwards)
- Quit - exits the program

Lastly, there are some miscellaneous features:

- A search box to cull the selectable variables
- A font size slider to control the text size on the plot
- Hoverable tooltips when the cursor is on a plot line
- A variable called *actual_iteration_number* that gives a translation between history file iteration number and run file iteration number. This is especially useful for debugging specific steps of an optimization or comparing values across different histories.

1.5.2 OptView-Dash

This is a [Dash](#) implementation of OptView, and has many of the same features offered by OptView. For installation instructions, see [Installing OptView](#). To run, use this command:

```
$ optview_dash <filename>
```

Similar to OptView, you can invoke it with multiple history files. To view the dash app, you will have to manually open the server in your browser that is listed in the terminal after running the above command.

Auto-refresh: This follows the same functionality as OptView, allowing you to see the changes of an optimization as it is running.

- If you toggle this checklist button, it will cause the program to default update every 10 seconds, however you may modify this refresh rate using the input box underneath
- Make sure to toggle off this button when you are done or the optimization is complete so it does not add lag.
- This feature also works with multiple history files/optimizations running!

1.5.3 Directly Accessing the History Object

The history file generated by pyOptSparse is just a SqliteDict object. To extract the stored information in Python, first initialize a History object:

```
hist = History("path/to/opt_hist.hst", flag="r")
```

From here, various information can be extracted, using the various `get_` methods. To extract iteration history, use the function `getValues()`. See the page [History](#) for a full description of the history file structure and the API.

1.6 Major changes compared to pyOpt

The following list summarizes some of the changes/improvements made to pyOpt to get pyOptSparse:

- Elimination of $\mathcal{O}(n^2)$ scaling behaviour when adding large numbers of design variables (>10,000)
- Proper handling of all optimizers when run in parallel environment (only a single optimization instance is run, not one instance per processor)
- More flexible return specification of constraints
- More flexible return specification of constraint *gradients*
- Complete elimination of gradient indexing errors using dictionary-based returns
- Substantial improvement of optimization script robustness through indexing elimination
- Automatic assembly of sparse Jacobians with both dense and sparse sub-blocks
- Automatic conversion of sparse Jacobian to dense for optimizers that cannot handle sparse constraints
- User specification of design variable scaling
- User specification of constraint scaling
- Design variable returns in dictionary format only
- Specification of linear constraints, dense or sparse
- Sparse non-linear Jacobians
- New history file format. Uses SQLite dictionaries.
- Fixed hot start bug where first call to user functions is a gradient. It is now guaranteed, that the first call is to the function evaluation, not the gradient.
- Various bug fixes in SNOPT
- Constraints can be in *any* order, independent of what the individual optimizer requires
- Python 3.x compatibility

1.7 How to Contribute to pyOptSparse

pyOptSparse is an open-source tool, thus we welcome users to submit additions or fixes to the code to make it better for everybody.

1.7.1 Issues

If you have an issue with pyOptSparse, a bug to report, or a feature to request, submit an issue on the GitHub repository. This lets other users know about the issue. If you are comfortable fixing the issue, please do so and submit a pull request.

1.7.2 Coding style

We use `black` for formatting. Please install it following its documentation, and run it with the command line argument `-l 120`, for example at the project root directory:

```
$ black . -l 120
```

This will automatically format all Python files.

We use `flake8` for linting. Please install it following its instructions, and run it at the project root with:

```
$ flake8 .
```

The configuration file we use for `flake8` is a combination of [this file](#) and the one at the root of this repository. If there are any PEP-8 violations, `flake8` will print out the nature of the violation. We run continuous integration with these tools on all pull requests submitted. For an easier workflow, we recommend integrating these tools with your code editor.

Warning: For a PR to be accepted, it must pass all GitHub checks, which include both formatting checks with `black` and syntax checks with `flake8`.

1.7.3 Documentation

When you add or modify code, make sure to provide relevant documentation that explains the new code. This should be done in code via docstrings and comments, but also in the Sphinx documentation as well if you add a new feature or capability. Look at the `.rst` files in the `doc` section of the repo.

To build documentation locally, go to the `doc` folder and type `make html`. Building the documentation requires `sphinx` and `numpydoc`, as well as the Sphinx RTD theme. To install these dependencies, type

```
$ pip install sphinx numpydoc sphinx-rtd-theme
```

1.7.4 Testing

When you add code or functionality, add tests that cover the new or modified code. These may be units tests for individual components or regression tests for entire models that use the new functionality. All the existing tests can be found under the `test` folder.

1.7.5 Pull requests

Finally, after adding or modifying code, and making sure the steps above are followed, submit a pull request via the GitHub interface. This will automatically go through all of the tests in the repo to make sure everything is functioning properly. The main developers of pyOptSparse will then merge in the request or provide feedback on how to improve the contribution.

1.8 pyOptSparse in published works

pyOptSparse has been used extensively in the field of engineering design optimization. The following is a non-exhaustive list of works that have used pyOptSparse. The citations are organized by the optimization framework for which pyOptSparse is used within.

1.8.1 MACH-Aero

MACH-Aero is an open-source aerodynamic shape optimization framework developed by the MDO Lab at the University of Michigan. Since the vast majority of publications from the MDO Lab uses the MACH framework (and as a result pyOptSparse), only a few select publications from the lab are listed below. The rest are works in conjunction with collaborators.

- Nathalie Bartoli, Mostafa Meliani, Joseph Morlier, Thierry Lefebvre, Mohamed-Amine Bouhlef, and Joaquim R. R. A. Martins. Multi-fidelity efficient global optimization: methodology and application to airfoil shape design. In *AIAA Aviation Forum*. June 2019. doi:10.2514/6.2019-3236.
- Nicolas P. Bons, Charles A. Mader, Joaquim R. R. A. Martins, Ana P. C. Cuco, and Felipe I. K. Odaguil. High-fidelity aerodynamic shape optimization of a full configuration regional jet. In *2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. Kissimmee, FL, January 2018. doi:10.2514/6.2018-0106.
- Nicolas P. Bons, Joaquim R. R. A. Martins, Charles A. Mader, Matthew McMullen, and Michelle Suen. High-fidelity aerostructural optimization studies of the Aerion AS2 supersonic business jet. In *Proceedings of the AIAA Aviation Forum*. June 2020. doi:10.2514/6.2020-3182.
- Benjamin J. Brelje, Joshua Anibal, Anil Yildirim, Charles A. Mader, and Joaquim R. R. A. Martins. Flexible formulation of spatial integration constraints in aerodynamic shape optimization. *AIAA Journal*, 58(6):2571–2580, June 2020. doi:10.2514/1.J058366.
- Timothy R. Brooks, Gaetan K. W. Kenway, and Joaquim R. R. A. Martins. Benchmark aerostructural models for the study of transonic aircraft wings. *AIAA Journal*, 56(7):2840–2855, July 2018. doi:10.2514/1.J056603.
- Timothy R. Brooks, Joaquim R. R. A. Martins, and Graeme J. Kennedy. High-fidelity aerostructural optimization of tow-steered composite wings. *Journal of Fluids and Structures*, 88:122–147, July 2019. doi:10.1016/j.jfluidstructs.2019.04.005.
- Timothy R. Brooks, Joaquim R. R. A. Martins, and Graeme J. Kennedy. Aerostructural trade-offs for tow-steered composite wings. *Journal of Aircraft*, 2020. doi:10.2514/1.C035699.
- David A. Burdette and Joaquim R. R. A. Martins. Impact of morphing trailing edge on mission performance for the Common Research Model. *Journal of Aircraft*, 56(1):369–384, January 2019. doi:10.2514/1.C034967.
- Gustavo L. O. Halila, Joaquim R. R. A. Martins, and Krzysztof J. Fidkowski. Adjoint-based aerodynamic shape optimization including transition to turbulence effects. *Aerospace Science and Technology*, pages 1–15, December 2020. doi:10.1016/j.ast.2020.106243.
- Ping He and Joaquim R. R. A. Martins. A hybrid time-spectral approach for aerodynamic shape optimization with unsteady flow. In *Proceedings of the AIAA SciTech Forum*. January 2021. doi:10.2514/6.2021-0278.

- Ping He, Grzegorz Filip, Joaquim R. R. A. Martins, and Kevin J. Maki. Design optimization for self-propulsion of a bulk carrier hull using a discrete adjoint method. *Computers & Fluids*, 192:104259, October 2019. doi:10.1016/j.compfluid.2019.104259.
- Ping He, Charles A. Mader, Joaquim R. R. A. Martins, and Kevin J. Maki. DAfoam: an open-source adjoint framework for multidisciplinary design optimization with OpenFOAM. *AIAA Journal*, March 2020. doi:10.2514/1.J058853.
- Xiaolong He, Jichao Li, Charles A. Mader, Anil Yildirim, and Joaquim R. R. A. Martins. Robust aerodynamic shape optimization—from a circle to an airfoil. *Aerospace Science and Technology*, 87:48–61, April 2019. doi:10.1016/j.ast.2019.01.051.
- Davide Ivaldi, Ney R. Secco, Song Chen, John T. Hwang, and Joaquim R. R. A. Martins. Aerodynamic shape optimization of a truss-braced-wing aircraft. In *Proceedings of the 16th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. Dallas, TX, June 2015. doi:10.2514/6.2015-3436.
- Jichao Li, Mohamed Amine Bouhlel, and Joaquim R. R. A. Martins. Data-based approach for fast airfoil analysis and optimization. *AIAA Journal*, 57(2):581–596, February 2019. doi:10.2514/1.J057129.
- Jichao Li, Sicheng He, and Joaquim R. R. A. Martins. Data-driven constraint approach to ensure low-speed performance in transonic aerodynamic shape optimization. *Aerospace Science and Technology*, 92:536–550, September 2019. doi:10.1016/j.ast.2019.06.008.
- Jichao Li, Mengqi Zhang, Joaquim R. R. A. Martins, and Chang Shu. Efficient aerodynamic shape optimization with deep-learning-based filtering. *AIAA Journal*, 58(10):4243–4259, October 2020. doi:10.2514/1.J059254.
- Zhoujie Lyu, Gaetan K. W. Kenway, and Joaquim R. R. A. Martins. Aerodynamic shape optimization investigations of the Common Research Model wing benchmark. *AIAA Journal*, 53(4):968–985, April 2015. doi:10.2514/1.J053318.
- Mads H. Aa. Madsen, Frederik Zahle, Niels N. Sørensen, and Joaquim R. R. A. Martins. Multipoint high-fidelity CFD-based aerodynamic shape optimization of a 10 MW wind turbine. *Wind Energy Science*, 4:163–192, April 2019. doi:10.5194/wes-4-163-2019.
- Ney R. Secco and Joaquim R. R. A. Martins. RANS-based aerodynamic shape optimization of a strut-braced wing with overset meshes. *Journal of Aircraft*, 56(1):217–227, January 2019. doi:10.2514/1.C034934.
- Yayun Shi, Charles A. Mader, Sicheng He, Gustavo L. O. Halila, and Joaquim R. R. A. Martins. Natural laminar-flow airfoil optimization design using a discrete adjoint approach. *AIAA Journal*, 58(11):4702–4722, November 2020. doi:10.2514/1.J058944.

1.8.2 OpenMDAO

OpenMDAO is a popular multidisciplinary design and optimization framework developed by NASA Glenn Research Center, and support pyOptSparse as one of the possible optimization drivers.

- Nathalie Bartoli, Thierry Lefebvre, Sylvain Dubreuil, Romain Olivanti, Nicolas Bons, Joaquim R. R. A. Martins, Mohamed Amine Bouhlel, and Joseph Morlier. An adaptive optimization strategy based on mixture of experts for wing aerodynamic design optimization. In *Proceedings of the 18th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. Denver, CO, June 2017. doi:10.2514/6.2017-4433.
- Alp Dener, Pengfei Meng, Jason E Hicken, Graeme Kennedy, John Hwang, and Justin S Gray. Kona: a parallel optimization library for engineering-design problems. In *57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, 1422. 2016. doi:10.2514/6.2016-1422.
- Justin S. Gray and Joaquim R. R. A. Martins. Coupled aeropropulsive design optimization of a boundary-layer ingestion propulsor. *The Aeronautical Journal*, 123(1259):121–137, January 2019. doi:10.1017/aer.2018.120.

- Tae H Ha, Keunseok Lee, and John T Hwang. Large-scale multidisciplinary optimization under uncertainty for electric vertical takeoff and landing aircraft. In *AIAA SciTech 2020 Forum*, 0904. 2020. doi:10.2514/6.2020-0904.
- John M. Hegseth, Erin E. Bachynski, and Joaquim R. R. A. Martins. Integrated design optimization of spar floating wind turbines. *Marine Structures*, 72:102771, July 2020. (Moan–Faltinsen Best Paper Award). doi:10.1016/j.marstruc.2020.102771.
- John Marius Hegseth, Erin E. Bachynski, and Joaquim R. R. A. Martins. Design optimization of spar floating wind turbines considering different control strategies. *Journal of Physics: Conference Series*, 1669:012010, October 2020. doi:10.1088/1742-6596/1669/1/012010.
- Austin J Herrema, Josef Kiendl, and Ming-Chen Hsu. A framework for isogeometric-analysis-based optimization of wind turbine blade structures. *Wind Energy*, 22(2):153–170, 2019. doi:10.1002/we.2276.
- Daniel Ingraham, Justin S Gray, and Leonard V Lopes. Gradient-based propeller optimization with acoustic constraints. In *AIAA SciTech 2019 Forum*, 1219. 2019. doi:10.2514/6.2019-1219.
- John Jasa, Benjamin Brelje, Justin Gray, Charles A. Mader, and Joaquim R. R. A. Martins. Large-scale path-dependent optimization of supersonic aircraft. *Aerospace*, October 2020. doi:10.3390/aerospace7100152.
- Graeme Kennedy and Yicong Fu. Topology optimization benchmark problems for assessing the performance of optimization algorithms. In *AIAA SciTech 2021 Forum*, 1357. 2021. doi:10.2514/6.2021-1357.
- Michael K. McWilliam, Frederik Zahle, Antariksh Dicholkar, David Verelst, and Taeseong Kim. Optimal aeroelastic design of a rotor with bend-twist coupling. *Journal of Physics: Conference Series*, 1037:042009, jun 2018. doi:10.1088/1742-6596/1037/4/042009.
- Rajaram Attukur Nandagopal and Srikanth Narasimalu. Multi-objective optimization of hydrofoil geometry used in horizontal axis tidal turbine blade designed for operation in tropical conditions of South East Asia. *Renewable Energy*, 146:166–180, 2020. doi:10.1016/j.renene.2019.05.111.
- A. S. Padrón, J. Thomas, A. P. J. Stanley, J. J. Alonso, and A. Ning. Polynomial chaos to efficiently compute the annual energy production in wind farm layout optimization. *Wind Energy Science*, 4(2):211–231, 2019. doi:10.5194/wes-4-211-2019.
- Christian Pavese, Carlo Tibaldi, Frederik Zahle, and Taeseong Kim. Aeroelastic multidisciplinary design optimization of a swept wind turbine blade. *Wind Energy*, 20(12):1941–1953, 2017. doi:10.1002/we.2131.
- Ignas Satkauskas, Evan Gaertner, Pietro Bortolotti, Garrett Barter, and Peter A Graf. Wind turbine rotor design optimization using importance sampling. In *AIAA SciTech 2020 Forum*, 1953. 2020. doi:10.2514/6.2020-1953.
- Jared J. Thomas and Andrew Ning. A method for reducing multi-modality in the wind farm layout optimization problem. In *Journal of Physics: Conference Series*, volume 1037. Milano, Italy, June 2018. The Science of Making Torque from Wind. doi:10.1088/1742-6596/1037/4/042012.
- Frederik Zahle, Carlo Tibaldi, Christian Pavese, Michael K. McWilliam, Jose P. A. A. Blasques, and Morten H. Hansen. Design of an aeroelastically tailored 10 MW wind turbine rotor. *Journal of Physics: Conference Series*, 753(6):062008, 2016.

OpenAeroStruct

OpenAeroStruct is a low-fidelity aerostructural optimization framework implemented in OpenMDAO, and as such can leverage the optimization capabilities of pyOptSparse.

- Timothy R Brooks and Benjamin D Smith. Aerostructural design optimization of the D8 aircraft using active aeroelastic tailoring. In *AIAA Scitech 2020 Forum*, 1967. 2020. doi:10.2514/6.2020-1967.
- Shamsheer S. Chauhan and Joaquim R. R. A. Martins. Low-fidelity aerostructural optimization of aircraft wings with a simplified wingbox model using OpenAeroStruct. In *Proceedings of the 6th International Conference on Engineering Optimization, EngOpt 2018*, 418–431. Lisbon, Portugal, September 2018. Springer. doi:10.1007/978-3-319-97773-7_38.
- John P. Jasa, Shamsheer S. Chauhan, Justin S. Gray, and Joaquim R. R. A. Martins. How certain physical considerations impact aerostructural wing optimization. In *AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. Dallas, TX, June 2019. doi:10.2514/6.2019-3242.
- John P. Jasa, John T. Hwang, and Joaquim R. R. A. Martins. Open-source coupled aerostructural optimization using Python. *Structural and Multidisciplinary Optimization*, 57(4):1815–1827, April 2018. doi:10.1007/s00158-018-1912-8.

1.8.3 SUAVE

SUAVE is a conceptual-level aircraft design framework developed at Stanford University that includes multiple analysis fidelities, and provides a pyOptSparse interface.

- Stanislav Karpuk and Ali Elham. Conceptual design trade study for an energy-efficient mid-range aircraft with novel technologies. In *AIAA Scitech 2021 Forum*, 0013. 2021. doi:10.2514/6.2021-0013.
- Michael Kruger and Alejandra Uranga. The feasibility of electric propulsion for commuter aircraft. In *AIAA Scitech 2020 Forum*, 1499. 2020. doi:10.2514/6.2020-1499.

1.8.4 Other

The works which did not use any of the aforementioned frameworks are listed here.

- N. Bartoli, T. Lefebvre, S. Dubreuil, R. Olivanti, R. Priem, N. Bons, Joaquim R. R. A. Martins, and J. Morlier. Adaptive modeling strategy for constrained global optimization with application to aerodynamic wing design. *Aerospace Science and Technology*, 90:85–102, July 2019. doi:10.1016/j.ast.2019.03.041.
- Julien de Mûelenaere and Juan J Alonso. High-fidelity trajectory based MDO for the conceptual design of an air-launched spaceplane. In *2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, 0416. 2018. doi:10.2514/6.2018-0416.
- John T Hwang, Arnav V Jain, and Tae H Ha. Large-scale multidisciplinary design optimization—review and recommendations. In *AIAA Aviation 2019 Forum*, 3106. 2019. doi:10.2514/6.2019-3106.
- Graeme J. Kennedy and Ting Wei Chin. A sequential convex optimization method for multimaterial compliance design problems. *Computers & Structures*, 212:110–124, 2019. doi:10.1016/j.compstruc.2018.10.007.
- Gaetan K. W. Kenway and Joaquim R. R. A. Martins. Multipoint high-fidelity aerostructural optimization of a transport aircraft configuration. *Journal of Aircraft*, 51(1):144–160, January 2014. doi:10.2514/1.C032150.
- Jichao Li and Jinsheng Cai. Massively multipoint aerodynamic shape design via surrogate-assisted gradient-based optimization. *AIAA Journal*, 58(5):1949–1963, 2020. doi:10.2514/1.J058491.
- Jichao Li, Jinsheng Cai, and Kun Qu. Drag reduction of transonic wings with surrogate-based optimization. In *Asia-Pacific International Symposium on Aerospace Technology*, 1065–1080. Springer, 2018. doi:10.1007/978-981-13-3305-7_85.

- Dev Rajnarayan, Andrew Ning, and Judd A. Mehr. Universal airfoil parametrization using b-splines. In *Proceedings of the AIAA Aviation Forum*. 2018. doi:10.2514/6.2018-3949.
- Smruti Sahoo, Xin Zhao, and Konstantinos Kyprianidis. A review of concepts, benefits, and challenges for future electrical propulsion-based aircraft. *Aerospace*, 7(4):44, 2020. doi:10.3390/aerospace7040044.

1.9 Citation

If you use pyOptSparse, please cite the following paper:

N. Wu, G. Kenway, C. A. Mader, J. Jasa, and J. R. R. A. Martins. pyOptSparse: A Python framework for large-scale constrained nonlinear optimization of sparse systems. *Journal of Open Source Software*, 5(54), 2564, October 2020. <https://doi.org/10.21105/joss.02564>

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```
@article{Wu2020,
  doi = {10.21105/joss.02564},
  year = {2020},
  publisher = {The Open Journal},
  volume = {5},
  number = {54},
  pages = {2564},
  author = {Neil Wu and Gaetan Kenway and Charles A. Mader and John Jasa and Joaquim R.
↪ R. A. Martins},
  title = {pyOptSparse: A Python framework for large-scale constrained nonlinear_
↪ optimization of sparse systems},
  journal = {Journal of Open Source Software}
}
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1.10.1 ALPSO

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```

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```
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```

```
<signature of Ty Coon>, 1 April 1989
Ty Coon, President of Vice
```

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 Modified for pyOpt - 2008, Ruben E. Perez (Ruben.Perez@rmc.ca)

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Patched for pyOpt - 2008, Ruben E. Perez (Ruben.Perez@rmc.ca)

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1.11 Optimization

class pyoptsparse.pyOpt_optimization.**Optimization**(*name, objFun, comm=None, sens=None*)

The main purpose of this class is to describe the structure and potentially, sparsity pattern of an optimization problem.

Parameters

name

[str] Name given to optimization problem.

objFun

[Python function handle] Function handle used to evaluate the objective function.

comm

[MPI intra communication] The communicator this problem will be solved on. This is required for both analysis when the objective is computed in parallel as well as to use the internal parallel gradient computations. Defaults to MPI.COMM_WORLD if not given.

sens

[str or python Function.] Specify method to compute sensitivities.

addCon(*name, *args, **kwargs*)

Convenience function. See addConGroup() for more information

addConGroup(*name, nCon, lower=None, upper=None, scale=1.0, linear=False, wrt=None, jac=None*)

Add a group of variables into a variable set. This is the main function used for adding variables to py-OptSparse.

Parameters

name

[str] Constraint name. All names given to constraints must be unique

nCon

[int] The number of constraints in this group

lower

[scalar or array] The lower bound(s) for the constraint. If it is a scalar, it is applied to all nCon constraints. If it is an array, the array must be the same length as nCon.

upper

[scalar or array] The upper bound(s) for the constraint. If it is a scalar, it is applied to all nCon constraints. If it is an array, the array must be the same length as nCon.

scale

[scalar or array] A scaling factor for the constraint. It is generally advisable to have most optimization constraint around the same order of magnitude.

linear

[bool] Flag to specify if this constraint is linear. If the constraint is linear, both the wrt and jac keyword arguments must be given to specify the constant portion of the constraint Jacobian.

The intercept term of linear constraints must be supplied as part of the bound information. The linear constraint $g_L \leq Ax + b \leq g_U$ is equivalent to $g_L - b \leq Ax \leq g_U - b$, and pyOptSparse requires the latter form. In this case, the arguments should be:

```
jac = {"dvName" : A, ...}, lower = gL - b, upper = gU - b
```

wrt

[iterable (list, set, OrderedDict, array etc)] ‘wrt’ stand for stands for ‘With Respect To’. This specifies for what dvs have non-zero Jacobian values for this set of constraints. The order is not important.

jac

[dictionary] For linear and sparse non-linear constraints, the constraint Jacobian must be passed in. The structure of jac dictionary is as follows:

```
{'dvName1':matrix1, 'dvName2', matrix1, ...}
```

They keys of the Jacobian must correspond to the dvGroups given in the wrt keyword argument. The dimensions of each “chunk” of the constraint Jacobian must be consistent. For example, matrix1 must have a shape of (nCon, nDvs) where nDVs is the total number of design variables in dvName1. matrix1 may be a dense numpy array or it may be scipy sparse matrix. However, it is *HIGHLY* recommended that sparse constraints are supplied to pyOptSparse using the pyOptSparse’s simplified sparse matrix format. The reason for this is that it is *impossible* for force scipy sparse matrices to keep a fixed sparsity pattern; if the sparsity pattern changes during an optimization, *IT WILL FAIL*.

The three simplified pyOptSparse sparse matrix formats are summarized below:

```
mat = {'coo':[row, col, data], 'shape':[nrow, ncols]} # A coo matrix
mat = {'csr':[rowp, colind, data], 'shape':[nrow, ncols]} # A csr_
↳matrix
mat = {'coo':[colp, rowind, data], 'shape':[nrow, ncols]} # A csc_
↳matrix
```

Note that for nonlinear constraints (`linear=False`), the values themselves in the matrices in `jac` do not matter, but the sparsity structure **does** matter. It is imperative that entries that will at some point have non-zero entries have non-zero entries in `jac` argument. That is, we do not let the sparsity structure of the Jacobian change throughout the optimization. This stipulation is automatically checked internally.

addObj(*name*, **args*, ***kwargs*)

Add Objective into Objectives Set

addVar(*name*, **args*, ***kwargs*)

This is a convenience function. It simply calls `addVarGroup()` with `nVars=1`. Variables added with `addVar()` are returned as *scalars*.

addVarGroup(*name*, *nVars*, *varType*='c', *value*=0.0, *lower*=None, *upper*=None, *scale*=1.0, *offset*=0.0, *choices*=[], ***kwargs*)

Add a group of variables into a variable set. This is the main function used for adding variables to `py-OptSparse`.

Parameters

name

[str] Name of variable group. This name should be unique across all the design variable groups

nVars

[int] Number of design variables in this group.

varType

[str.] String representing the type of variable. Suitable values for type are: 'c' for continuous variables, 'i' for integer values and 'd' for discrete selection.

value

[scalar or array.] Starting value for design variables. If it is a scalar, the same value is applied to all 'nVars' variables. Otherwise, it must be iterable object with length equal to 'nVars'.

lower

[scalar or array.] Lower bound of variables. Scalar/array usage is the same as value keyword

upper

[scalar or array.] Upper bound of variables. Scalar/array usage is the same as value keyword

scale

[scalar or array. Define a user supplied scaling] variable for the design variable group. This is often necessary when design variables of widely varying magnitudes are used within the same optimization. Scalar/array usage is the same as value keyword.

offset

[scalar or array. Define a user supplied offset] variable for the design variable group. This is often necessary when design variable has a large magnitude, but only changes a little about this value.

choices

[list] Specify a list of choices for discrete design variables

Notes

Calling `addVar()` and `addVarGroup(..., nVars=1, ...)` are **NOT** equivalent! The variable added with `addVar()` will be returned as scalar, while variable returned from `addVarGroup` will be an array of length 1.

It is recommended that the `addVar()` and `addVarGroup()` calls follow the examples above by including all the keyword arguments. This make it very clear the intent of the script's author. The type, value, lower, upper and scale should be given for all variables even if the default value is used.

Examples

```
>>> # Add a single design variable 'alpha'
>>> optProb.addVar('alpha', varType='c', value=2.0, lower=0.0, upper=10.0,
↳ scale=0.1)
>>> # Add 10 unscaled variables of 0.5 between 0 and 1 with name 'y'
>>> optProb.addVarGroup('y', varType='c', value=0.5, lower=0.0, upper=1.0,
↳ scale=1.0)
```

`checkConName(conName)`

Check if the desired constraint name has already been added. If it is has already been added, return a mangled name (a number appended) that *is* valid. This is intended to be used by classes that automatically add constraints to pyOptSparse.

Parameters

conName
[str] Constraint name to check validity on

Returns

validName
[str] A valid constraint name. May be the same as `conName` it that was, in fact, a valid name.

`checkVarName(varName)`

Check if the desired variable name `varName` if has already been added. If it is has already been added, return a mangled name (a number appended) that *is* valid. This is intended to be used by classes that automatically add variables to pyOptSparse

Parameters

varName
[str] Variable name to check validity on

Returns

validName
[str] A valid variable name. May be the same as `varName` it that was, in fact, a valid name.

`delVar(name)`

Delete a variable or variable group

Parameters

name
[str] Name of variable or variable group to remove

evaluateLinearConstraints(*x*, *fcon*)

This function is required for optimizers that do not explicitly treat the linear constraints. For those optimizers, we will evaluate the linear constraints here. We place the values of the linear constraints in the *fcon* dictionary such that it appears as if the user evaluated these constraints.

Parameters

x
[array] This must be the processed x-vector from the optimizer

fcon
[dict] Dictionary of the constraints. The linear constraints are to be added to this dictionary.

finalize()

This is a helper function which will only finalize the *optProb* if it's not already finalized.

getDVConIndex(*startIndex=1*, *printIndex=True*)

Return the index of a scalar DV/constraint, or the beginning and end index (inclusive) of a DV/constraint array. This is useful for looking at SNOPT gradient check output, and the default *startIndex=1* is for that purpose

getDVs()

Return a dictionary of the design variables. In most common usage, this function is not required.

Returns

outDVs
[dict] The dictionary of variables. This is the same as 'x' that would be used to call the user objective function.

getOrdering(*conOrder*, *oneSided*, *noEquality=False*)

Internal function that is used to produce a index list that reorders the constraints the way a particular optimizer needs.

Parameters

conOrder
[list] This must contain the following 4 strings: 'ni', 'li', 'ne', 'le' which stand for nonlinear inequality, linear inequality, nonlinear equality and linear equality. This defines the order that the optimizer wants the constraints

oneSided
[bool] Flag to do all constraints as one-sided instead of two sided. Most optimizers need this but some can deal with the two-sided constraints properly (snopt and ipopt for example)

noEquality
[bool] Flag to split equality constraints into two inequality constraints. Some optimizers (CONMIN for example) can't do equality constraints explicitly.

printSparsity(*verticalPrint=False*)

This function prints an (ASCII) visualization of the Jacobian sparsity structure. This helps the user visualize what pyOptSparse has been given and helps ensure it is what the user expected. It is highly recommended this function be called before the start of every optimization to verify the optimization problem setup.

Parameters

verticalPrint
[bool] True if the design variable names in the header should be printed vertically instead of horizontally. If true, this will make the constraint Jacobian print out more narrow and taller.

Warning: This function is **collective** on the optProb comm. It is therefore necessary to call this function on **all** processors of the optProb comm.

processConstraintJacobian(*gcon*)

This generic function is used to assemble the entire constraint Jacobian. The order of the constraint Jacobian is in ‘natural’ ordering, that is the order the constraints have been added (mostly; since it can be different when constraints are added on different processors).

The input is *gcon*, which is dict or an array. The array format should only be used when the pyOpt_gradient class is used since this results in a dense (and correctly oriented) Jacobian. The user should NEVER return a dense Jacobian since this extremely fickle and easy to break. The dict ‘*gcon*’ must contain only the non-linear constraints Jacobians; the linear ones will be added automatically.

Parameters

gcon

[array or dict] Constraint gradients. Either a complete 2D array or a nested dictionary of gradients given with respect to the variables.

Returns

gcon

[dict with csr data] Return the Jacobian in a sparse csr format. can be easily converted to csc, coo or dense format as required by individual optimizers

Warning: This function should not need to be called by the user

processContoDict(*fcon_in*, *scaled=True*, *dtype='d'*, *natural=False*, *multipliers=False*)

Parameters

fcon_in

[array] Array of constraint values to be converted into a dictionary

scaled

[bool] Flag specifying if the returned array should be scaled by the pyOpt scaling. The only type this is not true is when the automatic derivatives are used

dtype

[str] String specifying the data type to return. Normally this is ‘d’ for a float. The complex-step derivative computations will call this function with ‘D’ to ensure that the complex perturbations pass through correctly.

natural

[bool] Flag to specify if the input data is in the natural ordering. This is only used when computing gradient automatically with FD/CS.

multipliers

[bool] Flag that indicates whether this deprocessing is for the multipliers or the constraint values. In the case of multipliers, no constraint offset should be applied.

Warning: This function should not need to be called by the user

processContoVec(*fcon_in*, *scaled=True*, *dtype='d'*, *natural=False*)

Parameters**fcon_in**

[dict] Dictionary of constraint values

scaled

[bool] Flag specifying if the returned array should be scaled by the pyOpt scaling. The only type this is not true is when the automatic derivatives are used

dtype

[str] String specifying the data type to return. Normally this is 'd' for a float. The complex-step derivative computations will call this function with 'D' to ensure that the complex perturbations pass through correctly.

natural

[bool] Flag to specify if the data should be returned in the natural ordering. This is only used when computing gradient automatically with FD/CS.

Warning: This function should not need to be called by the user

processObjectiveGradient(*funcsSens*)

This generic function is used to assemble the objective gradient(s)

Parameters**funcsSens**

[dict] Dictionary of all function gradients. Just extract the objective(s) we need here.

Warning: This function should not need to be called by the user

processObjtoDict(*fobj_in, scaled=True*)

This function converts the objective in array form to the corresponding dictionary form.

Parameters**fobj_in**

[float or ndarray] The objective in array format. In the case of a single objective, a float can also be accepted.

scaled

[bool] Flag specifying if the returned dictionary should be scaled by the pyOpt scaling.

Returns**fobj**

[dictionary] The dictionary form of fobj_in, which is just a key:value pair for each objective.

processObjtoVec(*funcs, scaled=True*)

This is currently just a stub-function. It is here since in the future we may have to deal with multiple objectives so this function will deal with that

Parameters**funcs**

[dictionary of function values]

Returns

obj

[float or array] Processed objective(s).

Warning: This function should not need to be called by the user**processXtoDict**(*x*)

Take the flattened array of variables in ‘x’ and return a dictionary of variables keyed on the name of each variable.

Parameters**x**

[array] Flattened array from optimizer

Warning: This function should not need to be called by the user**processXtoVec**(*x*)

Take the dictionary form of x and convert back to flattened array.

Parameters**x**

[dict] Dictionary form of variables

Returns**x_array**

[array] Flattened array of variables

Warning: This function should not need to be called by the user**setDVs**(*inDVs*)

Set one or more groups of design variables from a dictionary. In most common usage, this function is not required.

Parameters**inDVs**

[dict] The dictionary of variables. The keys are the names of the variable groups, and the values are the desired design variable values for each variable group.

setDVsFromHistory(*histFile*, *key=None*)

Set optimization variables from a previous optimization. This is like a cold start, but some variables may have been added or removed from the previous optimization. This will try to set all variables it can.

Parameters**histFile**

[str] Filename of the history file to read

key

[str] Key of the history file to use for the x values. The default is None which will use the last x-value stored in the dictionary.

1.12 Optimizer

class pyoptsparse.pyOpt_optimizer.**Optimizer**(*args, **kwargs)

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

getInform(*infocode=None*)

Get optimizer result inform code at exit

Parameters

infocode

[int] Integer information code

getOption(*name*)

Return the optimizer option value for name

Parameters

name

[str] name of option for which to retrieve value

Returns

value

[varies] value of option for 'name'

setOption(*name, value=None*)

Generic routine for all option setting. The routine does error checking on the type of the value.

Parameters

name

[str] Name of the option to set

value

[varies] Variable value to set.

pyoptsparse.pyOpt_optimizer.**OPT**(*optName, *args, **kwargs*)

This is a simple utility function that enables creating an optimizer based on the 'optName' string. This can be useful for doing optimization studies with respect to optimizer since you don't need massive if-statements.

Parameters

optName

[str] String identifying the optimizer to create

***args, **kwargs**

[varies] Passed to optimizer creation.

Returns**opt**

[pyOpt_optimizer inherited optimizer] The desired optimizer

1.13 Gradient

class pyoptsparse.pyOpt_gradient.**Gradient**(*optProb, sensType, sensStep=None, sensMode='', comm=None*)

Gradient class for automatically computing gradients with finite difference or complex step.

Parameters**optProb**

[Optimization instance] This is the complete description of the optimization problem.

sensType

[str]

- FD for forward difference
- CD for central difference
- FDR for forward difference with relative step size
- CDR for central difference with relative step size
- CS for complex step

sensStep

[float] Step size to use for differencing

sensMode

[str] Flag to compute gradients in parallel.

1.14 Variable

class pyoptsparse.pyOpt_variable.**Variable**(*name, varType, value, lower, upper, scale, offset, scalar=False, choices=[]*)

This class holds the representation of a single pyOptSparse variable

See also:

[*pyoptsparse.pyOpt_optimization.Optimization.addVarGroup*](#)
for the full documentation

1.15 Constraint

class `pyoptsparse.pyOpt_constraint.Constraint`(*name, nCon, linear, wrt, jac, lower, upper, scale*)

This class holds the representation of a pyOptSparse constraint group

See also:

[`pyoptsparse.pyOpt_optimization.Optimization.addConGroup`](#)
for the full documentation

finalize(*variables, dvOffset, index*)

After the design variables have been finalized and the order is known we can check the constraint for consistency.

Parameters

variables

[OrderedDict] The pyOpt variable list after they have been finalized.

dvOffset

[dict] Design variable offsets from pyOpt_optimization

index

[int] The starting index of this constraint in natural order

Warning: This function should not need to be called by the user

1.16 Objective

class `pyoptsparse.pyOpt_objective.Objective`(*name, scale=1.0*)

This class holds the representation of a pyOptSparse objective.

Parameters

name

[str] Name of this objective

scale

[float] Scaling factor for objective. This does not change the actual optimization problem, but may be used to give a more human-meaningful value

See also:

[`pyoptsparse.pyOpt_optimization.Optimization.addObj`](#)
for the full documentation

1.17 Solution

class pyoptsparse.pyOpt_solution.**Solution**(*optProb, xStar, fStar, lambdaStar, optInform, info*)

This class is used to describe the solution of an optimization problem. This class inherits from Optimization which enables a solution to be used as an input to a subsequent optimization problem.

Parameters

optProb

[Optimization problem class] Optimization problem used to create solution

xStar

[dict] The final design variables

fStar

[dict] The final objective(s)

lambdaStar

[dict] The final Lagrange multipliers

optInform

[int] The inform code returned by the optimizer

info

[dict] A dictionary containing timing and call counter info to be stored in the Solution object.

1.18 History

Suppose we have an optimization problem with one DV group *xvars*, one constraint *con*, and the objective is called *obj*. In this case, the history file would have the following layout:



(continues on next page)



The main optimization history is indexed via call counters, in this example 0 and 1. Note that they do not match the major/minor iterations of a given optimizer, since gradient evaluations are stored separate from the function evaluation.

For SNOPT, a number of other values can be requested and stored in each major iteration, such as the feasibility and optimality from the SNOPT print out file.

1.18.1 API

class `pyoptsparse.pyOpt_history.History`(*fileName*, *optProb=None*, *temp=False*, *flag='r'*)

This class is essentially a thin wrapper around a SqliteDict dictionary to facilitate operations with pyOptSparse

Parameters

fileName

[str] File name for history file

optProb

[pyOpt_Optimization] The optimization object

temp

[bool] Flag to signify that the file should be deleted after it is closed

flag

[str] String specifying the mode. Similar to what was used in shelve. `n` for a new database and `r` to read an existing one.

close()

Close the underlying database. This should only be used in write mode. In read mode, we close the db during initialization.

getCallCounters()

Returns a list of all call counters stored in the history file.

Returns**list**

a list of strings, each entry being a call counter.

getConInfo(key=None)

Returns the *ConInfo*, for all keys by default. A *key* parameter can also be supplied, to retrieve *ConInfo* corresponding to specific constraints.

Parameters**key**

[str or list of str, optional] Specifies for which constraint to extract *ConInfo*.

Returns**dict**

A dictionary containing *ConInfo*. For a single key, the return is one level deeper.

getConNames()

Returns the names of constraints.

Returns**list of str**

A list containing the names of constraints.

getDVInfo(key=None)

Returns the *DVInfo*, for all keys by default. A *key* parameter can also be supplied, to retrieve *DVInfo* corresponding to specific DVs.

Parameters**key**

[str or list of str, optional] Specifies for which DV to extract *DVInfo*.

Returns**dict**

A dictionary containing *DVInfo*. For a single key, the return is one level deeper.

getDVNames()

Returns the names of the DVs.

Returns**list of str**

A list containing the names of DVs.

getExtraFuncsNames()

Returns extra funcs names. These are extra key: value pairs stored in the *funcs* dictionary for each iteration, which are not used by the optimizer.

Returns**list of str**

A list containing the names of extra funcs keys.

getIterKeys()

Returns the keys available at each optimization iteration. This function is useful for inspecting the history file, to determine what information is saved at each iteration.

Returns**list of str**

A list containing the names of keys stored at each optimization iteration.

getMetadata()

Returns a copy of the metadata stored in the history file.

Returns**dict**

A dictionary containing the metadata.

getObjInfo(key=None)

Returns the *ObjInfo*, for all keys by default. A *key* parameter can also be supplied, to retrieve *ObjInfo* corresponding to specific keys.

Parameters**key**

[str or list of str, optional] Specifies for which obj to extract *ObjInfo*.

Returns**dict**

A dictionary containing *ObjInfo*. For a single key, the return is one level deeper.

Notes

Recall that for the sake of generality, pyOptSparse allows for multiple objectives to be added. This feature is not used currently, but does make *ObjInfo* follow the same structure as *ConInfo* and *DVInfo*. Because of this, it is recommended that this function be accessed using the optional *key* argument.

getObjNames()

Returns the names of the objectives.

Returns**list of str**

A list containing the names of objectives.

Notes

Recall that for the sake of generality, pyOptSparse allows for multiple objectives to be added. This feature is not used currently, but does make *ObjNames* follow the same structure as *ConNames* and *DVNames*.

getOptProb()

Returns a copy of the *optProb* associated with the optimization.

Returns**optProb**

[pyOpt_optimization object] The *optProb* associated with the optimization. This is taken from the history file, and therefore has the *comm* and *objFun* fields removed.

getValues(*names=None, callCounters=None, major=True, scale=False, stack=False, allowSens=False*)

Parses an existing history file and returns a data dictionary used to post-process optimization results, containing the requested optimization iteration history.

Parameters

names

[list or str] the values of interest, can be the name of any DV, objective or constraint, or a list of them. If None, all values are returned. This includes the DVs, funcs, and any values stored by the optimizer.

callCounters

[list of ints, can also contain 'last'] a list of callCounters to extract information from. If the callCounter is invalid, i.e. outside the range or is a funcsSens evaluation, then it is skipped. 'last' represents the last major iteration. If None, values from all callCounters are returned.

major

[bool] flag to specify whether to include only major iterations.

scale

[bool] flag to specify whether to apply scaling for the values. True means to return values that are scaled the same way as the actual optimization.

stack

[bool] flag to specify whether the DV should be stacked into a single numpy array with the key *xuser*, or retain their separate DVGroups.

allowSens: bool

flag to specify whether gradient evaluation iterations are allowed. If true, it is up to the user to ensure that the callCounters specified contain the information requested.

Returns

dict

a dictionary containing the information requested. The keys of the dictionary correspond to the *names* requested. Each value is a numpy array with the first dimension equal to the number of callCounters requested.

Notes

Regardless of the major flag, failed function evaluations are not returned.

Examples

First we can request DV history over all major iterations:

```
>>> hist.getValues(names='xvars', major=True)
{'xvars': array([[ -2.00000000e+00,  1.00000000e+00],
 [ -1.00000000e+00,  9.00000000e-01],
 [ -5.00305827e-17,  4.21052632e-01],
 [  1.73666171e-06,  4.21049838e-01],
 [  9.08477459e-06,  4.21045261e-01],
 [  5.00000000e-01,  2.84786405e-01],
 [  5.00000000e-01,  5.57279939e-01],
 [  5.00000000e-01,  2.00000000e+00]])}
```

Next we can look at DV and optimality for the first and last iteration only:

```
>>> hist.getValues(names=['xvars','optimality'],callCounters=[0,'last'])
{'optimality': array([1.27895528, 0. ]),
 'xvars': array([[ -2. ,  1. ],
                [ 0.5,  2. ]])}
```

pointExists(callCounter)

Determine if callCounter is in the database

Parameters**callCounter**

[int or str of int]

Returns**bool**

True if the callCounter exists in the history file. False otherwise.

read(key)

Read data for an arbitrary key. Returns None if key is not found. If passing in a callCounter, it should be verified by calling pointExists() first.

Parameters**key**

[str or int] generic key[str] or callCounter[int]

Returns**dict**

The value corresponding to *key* is returned. If the key is not found, *None* is returned instead.

write(callCounter, data)

This is the main to write data. Basically, we just pass in the callCounter, the integer forming the key, and a dictionary which will be written to the key

Parameters**callCounter**

[int] the callCounter to write to

data

[dict] the dictionary corresponding to the callCounter

writeData(key, data)

Write arbitrary *key:data* value to db.

Parameters**key**

[str] The key to be added to the history file

data

The data corresponding to the key. It can be anything as long as it is serializable in *sqlite-dict*.

1.19 Utils

pyOptSparse_utils holds a minimal set of sparse-matrix type routines for pyOptSparse. This is designed to replace the SciPy sparse matrix formats, which have no way to enforce a constant sparsity structure as required by the optimizers. We use a very simple dictionary format to represent the three most common forms of sparse matrices:

```
mat = {'coo':[row, col, data], 'shape':[nrow, ncols]} # A coo matrix
mat = {'csr':[rowp, colind, data], 'shape':[nrow, ncols]} # A csr matrix
mat = {'csc':[colp, rowind, data], 'shape':[nrow, ncols]} # A csc matrix
```

pyoptsparse.pyOpt_utils.**convertToCOO**(mat)

Take a pyoptsparse sparse matrix definition of a COO, CSR or CSC matrix or numpy array or scipy sparse matrix and return the same matrix in COO format.

Parameters

mat

[dict or numpy array] A sparse matrix representation or numpy array

Returns

newMat

[dict] A coo representation of the same matrix

pyoptsparse.pyOpt_utils.**convertToCSC**(mat)

Take a pyoptsparse sparse matrix definition of a COO, CSR or CSC matrix or numpy array and return the same matrix in CSR format

Parameters

mat

[dict or numpy array] A sparse matrix representation or numpy array

Returns

newMat

[dict] A coo representation of the same matrix

pyoptsparse.pyOpt_utils.**convertToCSR**(mat)

Take a pyoptsparse sparse matrix definition of a COO, CSR or CSC matrix or numpy array and return the same matrix in CSR format

Parameters

mat

[dict or numpy array] A sparse matrix representation or numpy array

Returns

newMat

[dict] A coo representation of the same matrix

pyoptsparse.pyOpt_utils.**convertToDense**(mat)

Take a pyoptsparse sparse matrix definition and convert back to a dense format. This is typically the final step for optimizers with dense constraint jacobians.

Parameters

mat

[dict] A sparse matrix representation. Should be in CSR format for best efficiency

Returns

newMat

[array] A dense numpy array of the same matrix

`pyoptsparse.pyOpt_utils.extractRows(mat, indices)`

Extract the rows defined by 'indices' and return a new CSR matrix.

Parameters**mat**

[dict] pyoptsparse matrix CSR format

indices

[list/array of integer] The rows the user wants to extract

Returns**newMat**

[dic] pyoptsparse CSR matrix

`pyoptsparse.pyOpt_utils.mapToCSC(mat)`

Given a pyoptsparse matrix definition, return a tuple containing a map of the matrix to the CSC format.

Parameters**mat**

[dict] A sparse matrix representation.

Returns**tup**

[tuple of numpy arrays]

tup[0]

[numpy array (size=nnz)] An array that holds the row index of each element in the CSC representation of the data.

tup[1]

[numpy array (size=num_cols+1)] An array that holds the indices in the CSC representation and data at which each column begins. The last index of contains the number of nonzero elements in the sparse array.

tup[2]

[numpy array] An indexing array which maps the elements in the data array to elements in the CSC data array.

`pyoptsparse.pyOpt_utils.mapToCSR(mat)`

Given a pyoptsparse matrix definition, return a tuple containing a map of the matrix to the CSR format.

Parameters**mat**

[dict] A sparse matrix representation.

Returns**tup**

[tuple of numpy arrays]

tup[0]

[numpy array (size=num_rows+1)] An array that holds the indices in col_idx and data at which each row begins. The last index of contains the number of nonzero elements in the sparse array.

tup[1]

[numpy array (size=nnz)] An array of the column indices of each element in data.

tup[2]

[numpy array (size=nnz)] An indexing array which maps the elements in the data array to elements in the CSR data array.

`pyoptsparse.pyOpt_utils.scaleColumns(mat, factor)`

d= Scale the columns of the matrix. Must be CSR format

`pyoptsparse.pyOpt_utils.scaleRows(mat, factor)`

Scale the rows of the matrix. Must be CSR format

1.20 SNOPT

SNOPT is a sparse nonlinear optimizer that is particularly useful for solving large-scale constrained problems with smooth objective functions and constraints. The algorithm consists of a sequential quadratic programming (SQP) algorithm that uses a smooth augmented Lagrangian merit function, while making explicit provision for infeasibility in the original problem and in the quadratic programming subproblems. The Hessian of the Lagrangian is approximated using the BFGS quasi-Newton update.

1.20.1 Installation

SNOPT is available for purchase [here](#). Upon purchase, you should receive a zip file. Within the zip file, there is a folder called `src`. To use SNOPT with `pyoptsparse`, paste all files from `src` except `snoph.f` into `pyoptsparse/pySNOPT/source`.

From v2.0 onwards, only SNOPT v7.7.x is officially supported. To use `pyOptSparse` with previous versions of SNOPT, please checkout release v1.2. We currently test v7.7.7 and v7.7.1.

1.20.2 Options

Please refer to the SNOPT user manual for a complete listing of options and their default values. The following are a list of

- options which have values changed from the defaults within SNOPT
- options unique to `pyOptSparse`, implemented in the Python wrapper and not found in SNOPT

Table 1: SNOPT Default Options

Name	Type	Default value	Description
iPrint	int	18	Print File Output Unit (override internally in snopt?)
iSumm	int	19	Summary File Output Unit (override internally in snopt?)
Print file	str	SNOPT_print.out	Print file name
Summary file	str	SNOPT_summary.out	Summary file name
Minor print level	int	0	Minor iterations print level
Problem Type	str	Minimize	This specifies the problem type for SNOPT. <ul style="list-style-type: none"> • Minimize: minimization problem. • Maximize: maximization problem. • Feasible point: compute a feasible point only.
Start	str	Cold	This value is directly passed to the SNOPT kernel, and will be overwritten if another option, e.g. Cold start is supplied, in accordance with SNOPT options precedence. <ul style="list-style-type: none"> • Cold: Cold start • Hot: Hot start
Derivative level	int	3	The SNOPT derivative level. Only “3” is tested, where all derivatives are provided to SNOPT.
Iterations limit	int	10000000	The limit on the total number of minor iterations, summed over all major iterations. This option is set to a very large number to prevent premature termination of SNOPT.
Minor iterations limit	int	10000	The limit on the number of minor iterations <i>for each major iteration</i> . This option is set to a very large number to prevent premature termination of SNOPT.
Proximal iterations limit	int	10000	The iterations limit for solving the proximal point problem. We set this by default to a very large value in order to fully solve the proximal point problem to optimality
Total character	int	None	The total character

1.20.3 Informs

Table 2: SNOPT Informs

Code	Description
0	finished successfully
1	optimality conditions satisfied
2	feasible point found
3	requested accuracy could not be achieved
4	weak QP minimizer
10	the problem appears to be infeasible
11	infeasible linear constraints
12	infeasible linear equalities
13	nonlinear infeasibilities minimized
14	infeasibilities minimized
15	infeasible linear constraints in QP subproblem
20	the problem appears to be unbounded
21	unbounded objective
22	constraint violation limit reached
30	resource limit error
31	iteration limit reached
32	major iteration limit reached
33	the superbasics limit is too small
40	terminated after numerical difficulties
41	current point cannot be improved
42	singular basis
43	cannot satisfy the general constraints
44	ill-conditioned null-space basis
50	error in the user-supplied functions
51	incorrect objective derivatives
52	incorrect constraint derivatives
53	the QP Hessian is indefinite
54	incorrect second derivatives
55	incorrect derivatives
56	irregular or badly scaled problem functions
60	undefined user-supplied functions
61	undefined function at the first feasible point
62	undefined function at the initial point
63	unable to proceed into undefined region
70	user requested termination
71	terminated during function evaluation
72	terminated during constraint evaluation
73	terminated during objective evaluation
74	terminated from monitor routine
80	insufficient storage allocated
81	work arrays must have at least 500 elements
82	not enough character storage
83	not enough integer storage
84	not enough real storage
90	input arguments out of range
91	invalid input argument

continues on next page

Table 2 – continued from previous page

Code	Description
92	basis file dimensions do not match this problem
93	the QP Hessian is indefinite
100	finished successfully
101	SPECS file read
102	Jacobian structure estimated
103	MPS file read
104	memory requirements estimated
105	user-supplied derivatives appear to be correct
106	no derivatives were checked
107	some SPECS keywords were not recognized
110	errors while processing MPS data
111	no MPS file specified
112	problem-size estimates too small
113	fatal error in the MPS file
120	errors while estimating Jacobian structure
121	cannot find Jacobian structure at given point
130	fatal errors while reading the SP
131	no SPECS file (iSpecs le 0 or iSpecs gt 99)
132	End-of-file while looking for a BEGIN
133	End-of-file while reading SPECS file
134	ENDRUN found before any valid SPECS
140	system error
141	wrong no of basic variables
142	error in basis package

1.20.4 API

`class pyoptsparse.pySNOPT.pySNOPT.SNOPT(*args, **kwargs)`

SNOPT Optimizer Class - Inherited from Optimizer Abstract Class

SNOPT Optimizer Class Initialization

`__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True, timeLimit=None, restartDict=None)`

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. The default is None which will use SNOPT's own finite differences which are vastly superior to the pyOptSparse implementation. To explicitly use pyOptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as he requested evaluation point from SNOPT does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

timeLimit

[float] Specify the maximum amount of time for optimizer to run. Must be in seconds. This can be useful on queue systems when you want an optimization to cleanly finish before the job runs out of time.

restartDict

[dict] A dictionary containing the necessary information for hot-starting SNOPT. This is typically the same dictionary returned by this function on a previous invocation.

Returns**sol**

[Solution object] The optimization solution

restartDict

[dict] If 'Return work arrays' is True, a dictionary of arrays is also returned

1.21 IPOPT

IPOPT (Interior Point OPTimizer) is an open source interior point optimizer, designed for large-scale nonlinear optimization. The source code can be found [here](#). The latest version we support is 3.13.2.

1.21.1 Installation

IPOPT must be installed separately, then linked to pyOptSparse when building. For the full installation instructions, please see [their documentation](#). OpenMDAO also has a very helpful [script](#) which can be used to install IPOPT with other linear solvers. Here we explain a basic setup using MUMPS as the linear solver, together with METIS adapted from the OpenMDAO script.

1. Download the tarball and extract it to \$IPOPT_DIR which could be set to for example \$HOME/packages/Ipopt.
2. Install METIS, which can be used to improve the performance of the MUMPS linear solver.

```
# build METIS
cd $ILOPT_DIR
git clone https://github.com/coin-or-tools/ThirdParty-Metis.git
cd ThirdParty-Metis
./get.Metis
./configure --prefix=$ILOPT_DIR
make
make install
```

3. Install MUMPS

```
# build MUMPS
cd $ILOPT_DIR
git clone https://github.com/coin-or-tools/ThirdParty-Mumps.git
cd ThirdParty-Mumps
./get.Mumps
./configure --with-metis --with-metis-lflags="-L${ILOPT_DIR}/lib -lcoinmetis" \
  --with-metis-cflags="-I${ILOPT_DIR}/include -I${ILOPT_DIR}/include/coin-or -I$
↪ ${ILOPT_DIR}/include/coin-or/metis" \
  --prefix=$ILOPT_DIR CFLAGS="-I${ILOPT_DIR}/include -I${ILOPT_DIR}/include/coin-
↪ or -I${ILOPT_DIR}/include/coin-or/metis" \
  FCFLAGS="-I${ILOPT_DIR}/include -I${ILOPT_DIR}/include/coin-or -I${ILOPT_DIR}/
↪ include/coin-or/metis"
make
make install
```

4. Build IPOPT

```
# build IPOPT
cd $ILOPT_DIR
mkdir build
cd build
../configure --prefix=${ILOPT_DIR} --disable-java --with-mumps --with-mumps-lflags=
↪ "-L${ILOPT_DIR}/lib -lcoinmumps" \
  --with-mumps-cflags="-I${ILOPT_DIR}/include/coin-or/mumps"
make
make install
```

5. You must add the IPOPT library path to the LD_LIBRARY_PATH variable for things to work right. This could be done for example by adding the following to your .bashrc:

```
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$ILOPT_DIR/lib
```

Furthermore, the environment variable \$ILOPT_DIR must be set correctly in order to link to pyOptSparse. Alternatively, you can manually define the variables \$ILOPT_LIB and \$ILOPT_INC for the lib and include paths separately.

6. Now clean build pyOptSparse. Verify that IPOPT works by running the relevant tests.

Note: To get IPOPT working with pyOptSparse when using another linear solver, several things must be changed.

1. The setup.py file located in pyoptsparse/pyIPOPT must be updated accordingly. In particular, the libraries= line must be changed to reflect the alternate linear solver. For example, for HSL you need to replace coinmumps and coinmetis with coinhsl.

2. The option `linear_solver` in the options dictionary must be changed. The default value can be changed in `pyIPOPT.py` so that this option does not need to be manually set in every run script.

1.21.2 Options

Please refer to the [IPOPT website](#) for complete listing of options. The following are the options which are set by default within pyOptSparse. All other options take the default value with IPOPT unless specified by the user.

Table 3: IPOPT Default Options

Name	Type	Default value	Description
<code>print_level</code>	int	0	Printing level
<code>file_print_level</code>	int	5	Printing level for the output file
<code>sb</code>	str	yes	This is an undocumented option which suppresses the IPOPT header from being printed to screen every time.
<code>print_user_options</code>	bool	yes	Whether to print the user-modified options
<code>output_file</code>	str	IPOPT.out	The name of the output file from IPOPT
<code>linear_solver</code>	str	mumps	The linear solver used.

1.21.3 Informs

Table 4: IPOPT Informs

Code	Description
0	Solve Succeeded
1	Solved To Acceptable Level
2	Infeasible Problem Detected
3	Search Direction Becomes Too Small
4	Diverging Iterates
5	User Requested Stop
6	Feasible Point Found
-1	Maximum Iterations Exceeded
-2	Restoration Failed
-3	Error In Step Computation
-4	Maximum CpuTime Exceeded
-10	Not Enough Degrees Of Freedom
-11	Invalid Problem Definition
-12	Invalid Option
-13	Invalid Number Detected
-100	Unrecoverable Exception
-101	NonIpopt Exception Thrown
-102	Insufficient Memory
-199	Internal Error

1.21.4 API

`class pyoptsparse.pyIPOPT.pyIPOPT.IPOPT(*args, **kwargs)`

IPOPT Optimizer Class - Inherited from Optimizer Abstract Class

IPOPT Optimizer Class Initialization

```
__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True)
```

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use pyOptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.22 SLSQP

SLSQP optimizer is a sequential least squares programming algorithm which uses the Han-Powell quasi-Newton method with a BFGS update of the B-matrix and an L1-test function in the step-length algorithm. The optimizer uses a slightly modified version of Lawson and Hanson's NNLS nonlinear least-squares solver.

The version provided is the original source code from 1991 by Dieter Kraft.

1.22.1 Options

Table 5: SLSQP Default Options

Name	Type	Default value	Description
ACC	float	1e-06	Convergence Accuracy
MAXIT	int	500	Maximum Iterations
IPRINT	int	1	Output Level (<0 - None, 0 - Screen, 1 - File)
IOUT	int	60	Output Unit Number
IFILE	str	SLSQP.out	Output File Name

1.22.2 Informs

Table 6: SLSQP Informs

Code	Description
-1	Gradient evaluation required (g & a)
0	Optimization terminated successfully.
1	Function evaluation required (f & c)
2	More equality constraints than independent variables
3	More than 3*n iterations in LSQ subproblem
4	Inequality constraints incompatible
5	Singular matrix E in LSQ subproblem
6	Singular matrix C in LSQ subproblem
7	Rank-deficient equality constraint subproblem HFTI
8	Positive directional derivative for linesearch
9	Iteration limit exceeded

1.22.3 API

```
class pyoptsparse.pySLSQP.pySLSQP.SLSQP(*args, **kwargs)
```

SLSQP Optimizer Class - Inherited from Optimizer Abstract Class

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

```
__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True)
```

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use pyOptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point from SLSQP does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.23 NLPQLP

NLPQLP is a sequential quadratic programming (SQP) method which solves problems with smooth continuously differentiable objective function and constraints. The algorithm uses a quadratic approximation of the Lagrangian function and a linearization of the constraints. To generate a search direction a quadratic subproblem is formulated and solved. The line search can be performed with respect to two alternative merit functions, and the Hessian approximation is updated by a modified BFGS formula.

NLPQLP is a proprietary software, which can be obtained [here](#). The latest version supported is v4.2.2.

1.23.1 Options

Table 7: NLPQLP Default Options

Name	Type	Default value	Description
accuracy	float	1e-06	Convergence accuracy
accuracyQP	float	1e-14	Convergence accuracy for QP
stepMin	float	1e-06	Minimum step length
maxFun	int	20	Maximum Number of Function Calls During Line Search
maxIt	int	500	Maximum Number of Iterations
maxNM	int	1	Maximum stack size for non-monotone line search
rho	float	1.0	Factor scaling identify for IFAIL=2
iPrint	int	2	Output Level <ul style="list-style-type: none"> • 2: Major • 0: None • 1: Final • 3: Major/Minor • 4: Full
mode	int	0	Mode (0 - Normal Execution, 1 to 18 - See Manual)
iOut	int	6	Output Unit Number
lMerit	bool	True	Merit Function Type (True - L2 Augmented Penalty, False - L1 Penalty)
lQl	bool	False	QP Subproblem Solver (True - Quasi-Newton, False - Cholesky)
iFile	str	NLPQLP.out	Output File Name

1.23.2 Informs

Table 8: NLPQLP Informs

Code	Description
-2	Compute gradient values w.r.t. the variables stored in first column of X, and store them in DF and DG. Only derivatives for active constraints ACTIVE(J)=.TRUE. need to be computed.
-1	Compute objective fn and all constraint values subject the variables found in the first L columns of X, and store them in F and G.
0	The optimality conditions are satisfied.
1	The algorithm has been stopped after MAXIT iterations.
2	The algorithm computed an uphill search direction.
3	Underflow occurred when determining a new approximation matrix for the Hessian of the Lagrangian.
4	The line search could not be terminated successfully.
5	Length of a working array is too short. More detailed error information is obtained with IPRINT>0
6	There are false dimensions, for example M>MMAX, N>=NMAX, or MNN2<>M+N+N+2.
7	The search direction is close to zero, but the current iterate is still infeasible.
8	The starting point violates a lower or upper bound.
9	Wrong input parameter, i.e., MODE, LDL decomposition in D and C (in case of MODE=1), IPRINT, IOUT
10	Internal inconsistency of the quadratic subproblem, division by zero.
11	More than MAXFUN successive non-evaluable function calls.
100	The solution of the quadratic programming subproblem has been terminated with an error message and IFAIL is set to IFQL+100, where IFQL denotes the index of an inconsistent constraint.

1.23.3 API

```
class pyoptsparse.pyNLPQLP.pyNLPQLP.NLPQLP(*args, **kwargs)
```

NLPQL Optimizer Class - Inherited from Optimizer Abstract Class

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

```
__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True)
```

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use pyOptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point from NLPQL does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.24 NSGA2

This optimizer is a non-dominating sorting genetic algorithm that solves non-convex and non-smooth single and multiobjective optimization problems. The algorithm attempts to perform global optimization, while enforcing constraints using a tournament selection-based strategy

Warning: Currently, the Python wrapper does not catch exceptions. If there is **any** error in the user-supplied function, you will get a seg-fault and no idea where it happened. Please make sure the objective is without errors before trying to use nsga2.

1.24.1 Options

Table 9: NSGA2 Default Options

Name	Type	Default value	Description
PopSize	int	100	Population size
maxGen	int	1000	Maximum number of generations
pCross_real	float	0.6	Probability of crossover of real variables
pMut_real	float	0.2	Probability of mutation of real variables
eta_c	float	10.0	Distribution index for crossover
eta_m	float	20.0	Distribution index for mutation
pCross_bin	float	0.0	Probability of crossover of binary variable
pMut_bin	float	0.0	Probability of mutation of binary variables
PrintOut	int	1	Flag to turn on output to filename
seed	int	0	Random Number Seed (0 - Auto-Seed based on time clock)
xinit	int	0	Use Initial Solution Flag (0 - random population, 1 - use given solution)

1.24.2 API

`class pyoptsparse.pyNSGA2.pyNSGA2.NSGA2(*args, **kwargs)`

NSGA2 Optimizer Class - Inherited from Optimizer Abstract Class

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

`__call__(optProb, storeHistory=None, hotStart=None, **kwargs)`

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to “replay” for the optimization. The optimization problem used to generate the history file specified in ‘hotStart’ must be **IDENTICAL** to the currently supplied ‘optProb’. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as he requested evaluation point from NSGA2 does not match the history, function and gradient evaluations revert back to normal evaluations.

Notes

The kwargs are there such that the `sens=` argument can be supplied (but ignored here in `nsga2`)

1.25 PSQP

This optimizer implements a sequential quadratic programming method with a BFGS variable metric update

1.25.1 Options

Table 10: PSQP Default Options

Name	Type	Default value	Description
XMAX	float	1e+16	Maximum Stepsize
TOLX	float	1e-16	Variable Change Tolerance
TOLC	float	1e-06	Constraint Violation Tolerance
TOLG	float	1e-06	Lagrangian Gradient Tolerance
RPF	float	0.0001	Penalty Coefficient
MIT	int	1000	Maximum Number of Iterations
MFV	int	2000	Maximum Number of Function Evaluations
MET	int	2	Variable Metric Update (1 - BFGS, 2 - Hoshino)
MEC	int	2	Negative Curvature Correction (1 - None, 2 - Powell's Correction)
IPRINT	int	2	Output Level (0 - None, 1 - Final, 2 - Iter)
IOUT	int	6	Output Unit Number
IFILE	str	PSQP.out	Output File Name

1.25.2 Informs

Table 11: PSQP Informs

Code	Description
1	Change in design variable was less than or equal to tolerance
2	Change in objective function was less than or equal to tolerance
3	Objective function less than or equal to tolerance
4	Maximum constraint value is less than or equal to tolerance
11	Maximum number of iterations exceeded
12	Maximum number of function evaluations exceeded
13	Maximum number of gradient evaluations exceeded
-6	Termination criterion not satisfied, but obtained point is acceptable
-7	Positive directional derivative in line search
-8	Interpolation error in line search
-10	Optimization failed

1.25.3 API

`class pyoptsparse.pyPSQP.pyPSQP.PSQP(*args, **kwargs)`

PSQP Optimizer Class - Inherited from Optimizer Abstract Class

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

`__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True)`

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use py-OptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point from PSQP does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.26 ParOpt

ParOpt is a nonlinear interior point optimizer that is designed for large parallel design optimization problems with structured sparse constraints. ParOpt is open source and can be downloaded at <https://github.com/smdogroup/paropt>. Documentation and examples for ParOpt can be found at <https://smdogroup.github.io/paropt/>. The version of ParOpt supported is v2.0.2.

1.26.1 Installation

Please follow the instructions [here](#) to install ParOpt as a separate Python package. Make sure that the package is named `paropt` and the installation location can be found by Python, so that `from paropt import ParOpt` works within the pyOptSparse folder. This typically requires installing it in a location which is already present under `$PYTHONPATH` environment variable, or you can modify the `.bashrc` file and manually append the path.

1.26.2 Options

Please see the ParOpt documentation for all available options.

1.26.3 API

```
class pyoptsparse.pyParOpt.ParOpt.ParOpt(*args, **kwargs)
```

ParOpt optimizer class

ParOpt has the capability to handle distributed design vectors. This is not replicated here since pyOptSparse does not have the capability to handle this type of design problem.

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

```
__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None,
          storeSens=True)
```

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use py-OptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point from ParOpt does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.27 CONMIN

CONstrained function MINimization (CONMIN) is a gradient-based optimizer that uses the methods of feasible directions.

1.27.1 Options

Table 12: CONMIN Default Options

Name	Type	Default value	Description
ITMAX	int	10000	Maximum Number of Iterations
DELFUN	float	1e-06	Objective Relative Tolerance
DABFUN	float	1e-06	Objective Absolute Tolerance
ITRM	int	5	None
NFEASCT	int	20	None
IPRINT	int	4	Print Control (0 - None, 1 - Final, 2,3,4 - Debug)
IOUT	int	6	Output Unit Number
IFILE	str	CONMIN.out	Output File Name

1.27.2 API

`class pyoptsparse.pyCONMIN.pyCONMIN.CONMIN(*args, **kwargs)`

CONMIN Optimizer Class - Inherited from Optimizer Abstract Class

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

`__call__(optProb, sens=None, sensStep=None, sensMode=None, storeHistory=None, hotStart=None, storeSens=True)`

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

sens

[str or python Function.] Specify method to compute sensitivities. To explicitly use pyOptSparse gradient class to do the derivatives with finite differences use 'FD'. 'sens' may also be 'CS' which will cause pyOptSparse to compute the derivatives using the complex step method. Finally, 'sens' may be a python function handle which is expected to compute the sensitivities directly. For expensive function evaluations and/or problems with large numbers of design variables this is the preferred method.

sensStep

[float] Set the step size to use for design variables. Defaults to 1e-6 when sens is 'FD' and 1e-40j when sens is 'CS'.

sensMode

[str] Use 'pgc' for parallel gradient computations. Only available with mpi4py and each objective evaluation is otherwise serial

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to "replay" for the optimization. The optimization problem used to generate the history file specified in 'hotStart' must be **IDENTICAL** to the currently supplied 'optProb'. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as the requested evaluation point from CONMIN does not match the history, function and gradient evaluations revert back to normal evaluations.

storeSens

[bool] Flag specifying if sensitivities are to be stored in hist. This is necessary for hot-starting only.

1.28 ALPSO

Augmented Lagrangian Particle Swarm Optimizer (ALPSO) is a PSO method that uses the augmented Lagrangian approach to handle constraints.

1.28.1 Options

Table 13: ALPSO Default Options

Name	Type	Default value	Description
SwarmSize	int	40	Number of Particles (Depends on Problem dimensions)
maxOuterIter	int	200	Maximum Number of Outer Loop Iterations (Major Iterations)
maxInnerIter	int	6	Maximum Number of Inner Loop Iterations (Minor Iterations)
minInnerIter	int	6	Minimum Number of Inner Loop Iterations (Dynamic Inner Iterations)
dynInnerIter	int	0	Dynamic Number of Inner Iterations Flag
stopCriteria	int	1	Stopping Criteria Flag (0 - maxIters, 1 - convergence)
stopIters	int	5	Consecutive Number of Iterations for which the Stopping Criteria must be Satisfied
etol	float	0.001	Absolute Tolerance for Equality constraints
itol	float	0.001	Absolute Tolerance for Inequality constraints
rtol	float	0.01	Relative Tolerance for Lagrange Multipliers
atol	float	0.01	Absolute Tolerance for Lagrange Function
dtol	float	0.1	Relative Tolerance in Distance of All Particles to Terminate (GCPSO)
printOuterIters	int	0	Number of Iterations Before Print Outer Loop Information
printInnerIters	int	0	Number of Iterations Before Print Inner Loop Information
rinit	float	1.0	Initial Penalty Factor
xinit	int	0	Initial Position Flag (0 - no position, 1 - position given)

continues on next page

Table 13 – continued from previous page

Name	Type	Default value	Description
vinit	float	1.0	Initial Velocity of Particles in Normalized [-1, 1] Design Space
vmax	float	2.0	Maximum Velocity of Particles in Normalized [-1, 1] Design Space
c1	float	2.0	Cognitive Parameter
c2	float	1.0	Social Parameter
w1	float	0.99	Initial Inertia Weight
w2	float	0.55	Final Inertia Weight
ns	int	15	Number of Consecutive Successes in Finding New Best Position of Best Particle Before Search Radius will be Increased (GCPSO)
nf	int	5	Number of Consecutive Failures in Finding New Best Position of Best Particle Before Search Radius will be Increased (GCPSO)
dt	float	1.0	Time step
vcrazy	float	0.0001	Craziness Velocity (Added to Particle Velocity After Updating the Penalty Factors and Langangian Multipliers)
fileout	int	1	Flag to Turn On Output to filename
filename	str	ALPSO.out	We could probably remove fileout flag if filename or fileinstance is given
seed	int	0	Random Number Seed (0 - Auto-Seed based on time clock)
HoodSize	int	40	Number of Neighbours of Each Particle
HoodModel	str	gbest	Neighbourhood Model (dl/srling - Double/Single Link Ring, wheel - Wheel, Spatial - based on spatial distance, sfrac - Spatial Fraction)
HoodSelf	int	1	Selfless Neighbourhood Model (0 - Include Particle i in NH i, 1 - Don't Include Particle i)

continues on next page

Table 13 – continued from previous page

Name	Type	Default value	Description
Scaling	int	1	Design Variables Scaling Flag (0 - no scaling, 1 - scaling between [-1, 1])
parallelType	str	None	Type of parallelization <ul style="list-style-type: none"> • None: No parallel function evaluations • EXT: Use parallel function evaluations

1.28.2 API

class pyoptsparse.pyALPSO.pyALPSO.**ALPSO**(*args, **kwargs)

ALPSO Optimizer Class - Inherited from Optimizer Abstract Class

*Keyword arguments:**

- pll_type -> STR: ALPSO Parallel Implementation (None, SPM- Static, DPM- Dynamic, POA-Parallel Analysis), *Default* = None

This is the base optimizer class that all optimizers inherit from. We define common methods here to avoid code duplication.

Parameters

name

[str] Optimizer name

category

[str] Typically local or global

defaultOptions

[dictionary] A dictionary containing the default options

informs

[dict] Dictionary of the inform codes

__call__(*optProb*, *storeHistory=None*, *hotStart=None*, **kwargs)

This is the main routine used to solve the optimization problem.

Parameters

optProb

[Optimization or Solution class instance] This is the complete description of the optimization problem to be solved by the optimizer

storeHistory

[str] File name of the history file into which the history of this optimization will be stored

hotStart

[str] File name of the history file to “replay” for the optimization. The optimization problem used to generate the history file specified in ‘hotStart’ must be **IDENTICAL** to the currently supplied ‘optProb’. By identical we mean, **EVERY SINGLE PARAMETER MUST BE IDENTICAL**. As soon as he requested evaluation point from ALPSO does not match the history and function evaluations revert back to normal evaluations.

Notes

The kwargs are there such that the `sens=` argument can be supplied (but ignored here in `alps0`)

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