Numdifftools Documentation

Release 0.9.41

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Nov 11, 2022

CONTENTS:

This is the documentation of **Numdifftools** version 0.9.41 released Nov 11, 2022.

Bleeding edge available at: https://github.com/pbrod/numdifftools.

Official releases are available at: http://pypi.python.org/pypi/Numdifftools.

CHAPTER

ONE

INTRODUCTION

1.1 What is numdifftools?

Numdifftools is a suite of tools written in _Python[5] to solve automatic numerical differentiation problems in one or more variables. Finite differences are used in an adaptive manner, coupled with a Richardson extrapolation methodology to provide a maximally accurate result. The user can configure many options like; changing the order of the method or the extrapolation, even allowing the user to specify whether complex-step, central, forward or backward differences are used.

The methods provided are:

- **Derivative**: Compute the derivatives of order 1 through 10 on any scalar function.
- **directionaldiff**: Compute directional derivative of a function of n variables
- **Gradient**: Compute the gradient vector of a scalar function of one or more variables.
- **Jacobian**: Compute the Jacobian matrix of a vector valued function of one or more variables.
- **Hessian**: Compute the Hessian matrix of all 2nd partial derivatives of a scalar function of one or more variables.
- **Hessdiag**: Compute only the diagonal elements of the Hessian matrix

All of these methods also produce error estimates on the result.

Numdifftools also provide an easy to use interface to derivatives calculated with in _AlgoPy[6]. Algopy stands for Algorithmic Differentiation in Python. The purpose of AlgoPy is the evaluation of higher-order derivatives in the *forward* and *reverse* mode of Algorithmic Differentiation (AD) of functions that are implemented as Python programs.

1.2 How the documentation is organized

Numdifftools has a lot of documentation. A high-level overview of how it's organized will help you know where to look for certain things:

- *Tutorials* (page 5) take you by the hand through a series of steps to load a CDF container and explore its contents or to construct a new dataset and validate it. Start here if you're new to numdifftools.
- *Topic guides* (page 19) discuss key topics and concepts at a fairly high level and provide useful background information and explanation.
- *Reference guides* (page 27) contain technical reference for APIs and other aspects of numdifftools' machinery. They describe how it works and how to use it but assume that you have a basic understanding of key concepts.
- *How-to guides* (page 15) are recipes. They guide you through the steps involved in addressing key problems and use-cases. They are more advanced than tutorials and assume some knowledge of how numdifftools works.

[5] http://www.python.org/
[6] https://pythonhosted.org/algopy/

CHAPTER

TWO

TUTORIALS

The pages in this section of the documentation are aimed at the newcomer to numdifftools. They're designed to help you get started quickly, and show how easy it is to work with numdifftools as a developer who wants to customise it and get it working according to their own requirements.

These tutorials take you step-by-step through some key aspects of this work. They're not intended to explain the *topics in depth* (page 19), or provide *reference material* (page 27), but they will leave you with a good idea of what it's possible to achieve in just a few steps, and how to go about it.

Once you're familiar with the basics presented in these tutorials, you'll find the more in-depth coverage of the same topics in the *How-to* (page 15) section.

The tutorials follow a logical progression, starting from installation of numdifftools and the creation of a brand new project, and build on each other, so it's recommended to work through them in the order presented here.

2.1 Install guide

Before you can use numdifftools, you'll need to get it installed. This guide will guide you through a simple installation that'll work while you walk through the introduction.

2.1.1 Install Python

Being a Python library, numdifftools requires Python. Preferably you ned version 3.4 or newer, but you get the latest version of Python at https://www.python.org/downloads/.

You can verify that Python is installed by typing `python` from the command shell; you should see something like:

```
Python 3.6.3 (64-bit)| (default, Oct 15 2017, 03:27:45)
[MSC v.1900 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

`pip` is the Python installer. Make sure yours is up-to-date, as earlier versions can be less reliable:

```
$ pip install --upgrade pip
```

2.1.2 Dependencies

Numdifftools requires numpy 1.9 or newer, scipy 0.8 or newer, and Python 2.7 or 3.3 or newer. This tutorial assumes you are using Python 3. Optionally you may also want to install Algopy 0.4 or newer and statsmodels 0.6 or newer in order to be able to use the easy to use interfaces to their derivative functions.

2.1.3 Install numdifftools

To install numdifftools simply type in the 'command' shell:

```
$ pip install numdifftools
```

to get the lastest stable version. Using pip also has the advantage that all requirements are automatically installed.

2.1.4 Verifying installation

To verify that numdifftools can be seen by Python, type `python` from your shell. Then at the Python prompt, try to import numdifftools:

```
>>> import numdifftools as nd
>>> print(nd.__version__)
0.9.41
```

To test if the toolbox is working correctly paste the following in an interactive python prompt:

```
nd.test('--doctest-module')
```

If the result show no errors, you now have installed a fully functional toolbox. Congratulations!

2.1.5 That's it!

That's it – you can now *move onto the getting started tutorial* (page 6)

2.2 Getting started

2.2.1 The derivative

How does numdifftools.Derivative work in action? A simple nonlinear function with a well known derivative is e^x. At $x = 0$, the derivative should be 1.

```
>>> import numpy as np
>>> from numpy import exp
>>> import numdifftools as nd
>>> f = nd.Derivative(exp, full_output=True)
>>> val, info = f(0)
>>> np.allclose(val, 1)
True
```

```
>>> np.allclose(info.error_estimate, 5.28466160e-14)
True
```

A second simple example comes from trig functions. The first four derivatives of the sine function, evaluated at $x = 0$, should be respectively $[cos(0), -sin(0), -cos(0), sin(0)]$, or $[1, 0, -1, 0]$.

```
>>> from numpy import sin
>>> import numdifftools as nd
>>> df = nd.Derivative(sin, n=1)
>>> np.allclose(df(0), 1.)
True
```

```
>>> ddf = nd.Derivative(sin, n=2)
>>> np.allclose(ddf(0), 0.)
True
```

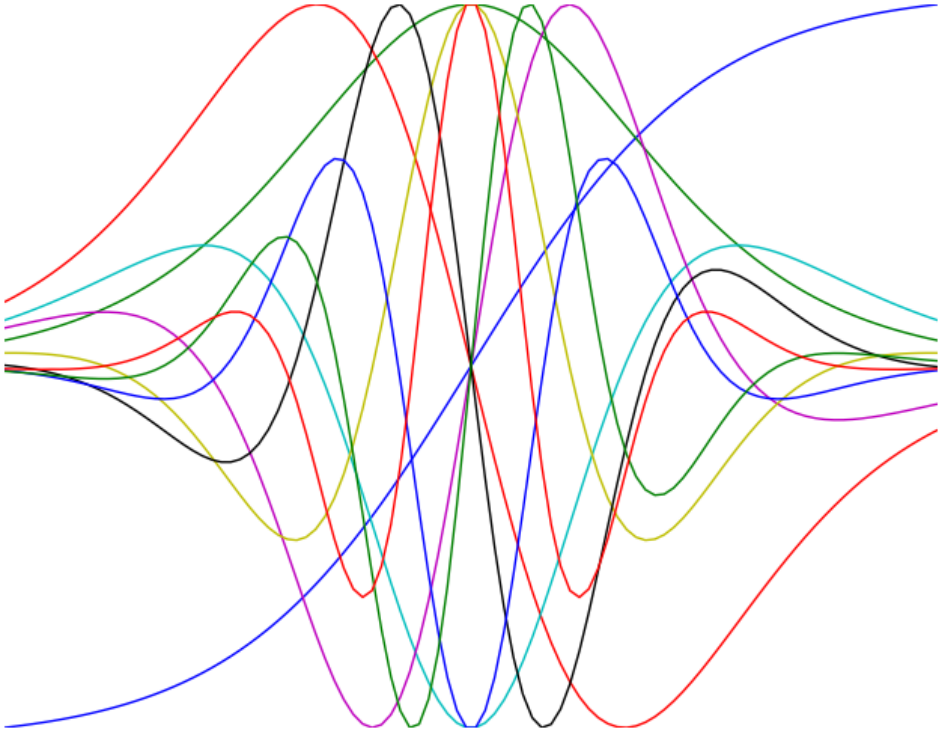
```
>>> dddf = nd.Derivative(sin, n=3)
>>> np.allclose(dddf(0), -1.)
True
```

```
>>> ddddf = nd.Derivative(sin, n=4)
>>> np.allclose(ddddf(0), 0.)
True
```

Visualize high order derivatives of the tanh function

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> x = np.linspace(-2, 2, 100)
>>> for i in range(10):
...     df = nd.Derivative(np.tanh, n=i)
...     y = df(x)
...     h = plt.plot(x, y/np.abs(y).max())
```

plt.show()



[7]

2.2.2 Gradient and Hessian estimation

Estimation of the gradient vector (numdifftools.Gradient) of a function of multiple variables is a simple task, requiring merely repeated calls to numdifftools.Derivative. Likewise, the diagonal elements of the hessian matrix are merely pure second partial derivatives of a function. numdifftools.Hessdiag accomplishes this task, again calling numdifftools.Derivative multiple times. Efficient computation of the off-diagonal (mixed partial derivative) elements of the Hessian matrix uses a scheme much like that of numdifftools.Derivative, then Richardson extrapolation is used to improve a set of second order finite difference estimates of those mixed partials.

[7] https://github.com/pbrod/numdifftools/blob/master/examples/fun.py

2.2.2.1 Multivariate calculus examples

Typical usage of the gradient and Hessian might be in optimization problems, where one might compare an analytically derived gradient for correctness, or use the Hessian matrix to compute confidence interval estimates on parameters in a maximum likelihood estimation.

2.2.2.2 Gradients and Hessians

```
>>> import numpy as np
>>> def rosen(x): return (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
```

Gradient of the Rosenbrock function at [1,1], the global minimizer

```
>>> grad = nd.Gradient(rosen)([1, 1])
```

The gradient should be zero (within floating point noise)

```
>>> np.allclose(grad, 0)
True
```

The Hessian matrix at the minimizer should be positive definite

```
>>> H = nd.Hessian(rosen)([1, 1])
```

The eigenvalues of H should be positive

```
>>> li, U = np.linalg.eig(H)
>>> [ val>0 for val in li]
[True,  True]
```

Gradient estimation of a function of 5 variables

```
>>> f = lambda x: np.sum(x**2)
>>> grad = nd.Gradient(f)(np.r_[1, 2, 3, 4, 5])
>>> np.allclose(grad, [  2.,   4.,   6.,   8.,  10.])
True
```

Simple Hessian matrix of a problem with 3 independent variables

```
>>> f = lambda x: x[0] + x[1]**2 + x[2]**3
>>> H = nd.Hessian(f)([1, 2, 3])
>>> np.allclose(H, np.diag([0, 2, 18]))
True
```

A semi-definite Hessian matrix

```
>>> H = nd.Hessian(lambda xy: np.cos(xy[0] - xy[1]))([0, 0])
```

one of these eigenvalues will be zero (approximately)

```
>>> [abs(val) < 1e-12 for val in np.linalg.eig(H)[0]]
[True, False]
```

2.2.2.3 Directional derivatives

The directional derivative will be the dot product of the gradient with the (unit normalized) vector. This is of course possible to do with numdifftools and you could do it like this for the Rosenbrock function at the solution, x0 = [1,1]:

```
>>> v = np.r_[1, 2]/np.sqrt(5)
>>> x0 = [1, 1]
>>> directional_diff = np.dot(nd.Gradient(rosen)(x0), v)
```

This should be zero.

```
>>> np.allclose(directional_diff, 0)
True
```

Ok, its a trivial test case, but it easy to compute the directional derivative at other locations:

```
>>> v2 = np.r_[1, -1]/np.sqrt(2)
>>> x2 = [2, 3]
>>> directionaldiff = np.dot(nd.Gradient(rosen)(x2), v2)
>>> np.allclose(directionaldiff, 743.87633380824832)
True
```

There is a convenience function $nd.directionaldiff$ that also takes care of the direction normalization:

```
>>> v = [1, -1]
>>> x0 = [2, 3]
>>> directional_diff = nd.directionaldiff(rosen, x0, v)
>>> np.allclose(directional_diff, 743.87633380824832)
True
```

2.2.2.4 Jacobian matrix

Jacobian matrix of a scalar function is just the gradient

```
>>> jac = nd.Jacobian(rosen)([2, 3])
>>> grad = nd.Gradient(rosen)([2, 3])
>>> np.allclose(jac, grad)
True
```

Jacobian matrix of a linear system will reduce to the design matrix

```
>>> A = np.random.rand(5,3)
>>> b = np.random.rand(5)
>>> fun = lambda x: np.dot(x, A.T) - b
>>> x = np.random.rand(3)
>>> jac = nd.Jacobian(fun)(x)
```

This should be essentially zero at any location x

```
>>> np.allclose(jac - A, 0)
True
```

The jacobian matrix of a nonlinear transformation of variables evaluated at some arbitrary location [-2, -3]

```
>>> fun = lambda xy: np.r_[xy[0]**2, np.cos(xy[0] - xy[1])]
>>> jac = nd.Jacobian(fun)([-2, -3])
>>> np.allclose(jac, [[-4.,  0.],
```

(continues on next page)

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```
...                   [-0.84147098,  0.84147098]])
True
```

2.3 Conclusion

numdifftools.Derivative is an a adaptive scheme that can compute the derivative of arbitrary (well behaved) functions. It is reasonably fast as an adaptive method. Many options have been provided for the user who wishes the ultimate amount of control over the estimation.

2.4 What to read next

So you've read all the *introductory material* (page 5) and have decided you'd like to keep using numdifftools. We've only just scratched the surface with this intro.

So what's next?

Well, we've always been big fans of learning by doing. At this point you should know enough to start a project of your own and start fooling around. As you need to learn new tricks, come back to the documentation.

We've put a lot of effort into making numdifftools's documentation useful, easy to read and as complete as possible. The rest of this document explains more about how the documentation works so that you can get the most out of it.

2.4.1 Finding documentation

Numdifftools got a *lot* of documentation, so finding what you need can sometimes be tricky. A few good places to start are the search and the genindex.

Or you can just browse around!

2.4.2 How the documentation is organized

Numdifftools main documentation is broken up into "chunks" designed to fill different needs:

- The *introductory material* (page 5) is designed for people new to numdifftools. It doesn't cover anything in depth, but instead gives a hands on overview of how to use numdifftools.
- The *topic guides* (page 19), on the other hand, dive deep into individual parts of numdifftools from a theoretical perspective.
- We've written a set of *how-to guides* (page 15) that answer common "How do I . . . ?" questions.
- The guides and how-to's don't cover every single class, function, and method available in numdifftools – that would be overwhelming when you're trying to learn. Instead, details about individual classes, functions, methods, and modules are kept in the *reference* (page 27). This is where you'll turn to find the details of a particular function or whatever you need.

2.4.3 How documentation is updated

Just as the numdifftools code base is developed and improved on a daily basis, our documentation is consistently improving. We improve documentation for several reasons:

- To make content fixes, such as grammar/typo corrections.
- To add information and/or examples to existing sections that need to be expanded.
- To document numdifftools features that aren't yet documented. (The list of such features is shrinking but exists nonetheless.)
- To add documentation for new features as new features get added, or as numdifftools APIs or behaviors change.

2.4.3.1 In plain text

For offline reading, or just for convenience, you can read the numdifftools documentation in plain text.

If you're using an official release of numdifftools, the zipped package (tarball) of the code includes a `docs/` directory, which contains all the documentation for that release.

If you're using the development version of numdifftools (aka the master branch), the `docs/` directory contains all of the documentation. You can update your Git checkout to get the latest changes.

One low-tech way of taking advantage of the text documentation is by using the Unix `grep` utility to search for a phrase in all of the documentation. For example, this will show you each mention of the phrase "max_length" in any numdifftools document:

```
$ grep -r max_length /path/to/numdifftools/docs/
```

2.4.3.2 As HTML, locally

You can get a local copy of the HTML documentation following a few easy steps:

- numdifftools's documentation uses a system called Sphinx[8] to convert from plain text to HTML. You'll need to install Sphinx by either downloading and installing the package from the Sphinx website, or with `pip`:

  ```
  $ pip install Sphinx
  ```

- Then, just use the included `Makefile` to turn the documentation into HTML:

  ```
  $ cd path/to/numdifftools/docs
  $ make html
  ```

  You'll need GNU Make[9] installed for this.

  If you're on Windows you can alternatively use the included batch file:

  ```
  $ cd path\to\numdifftools\docs
  $ make.bat html
  ```

- The HTML documentation will be placed in `docs/_build/html`.

[8] http://sphinx-doc.org/
[9] https://www.gnu.org/software/make/

2.4.3.3 Using pydoc

The pydoc module automatically generates documentation from Python modules. The documentation can be presented as pages of text on the console, served to a Web browser, or saved to HTML files.

For modules, classes, functions and methods, the displayed documentation is derived from the docstring (i.e. the __doc__ attribute) of the object, and recursively of its documentable members. If there is no docstring, pydoc tries to obtain a description from the block of comment lines just above the definition of the class, function or method in the source file, or at the top of the module (see inspect.getcomments()).

The built-in function help() invokes the online help system in the interactive interpreter, which uses pydoc to generate its documentation as text on the console. The same text documentation can also be viewed from outside the Python interpreter by running pydoc as a script at the operating system's command prompt. For example, running

```
$ pydoc numdifftools
```

at a shell prompt will display documentation on the numdifftools module, in a style similar to the manual pages shown by the Unix man command. The argument to pydoc can be the name of a function, module, or package, or a dotted reference to a class, method, or function within a module or module in a package. If the argument to pydoc looks like a path (that is, it contains the path separator for your operating system, such as a slash in Unix), and refers to an existing Python source file, then documentation is produced for that file.

You can also use pydoc to start an HTTP server on the local machine that will serve documentation to visiting Web browsers. For example, running

```
$ pydoc -b
```

will start the server and additionally open a web browser to a module index page. Each served page has a navigation bar at the top where you can Get help on an individual item, Search all modules with a keyword in their synopsis line, and go to the Module index, Topics and Keywords pages. To quit the server just type

```
$ quit
```

See also:

Numdifftools is 100% Python[10], so if you're new to Python[11], you might want to start by getting an idea of what the language is like. Below we have given some pointers to some resources you can use to get acquainted with the language.

If you're new to programming entirely, you might want to start with this list of Python resources for non-programmers[12]

If you already know a few other languages and want to get up to speed with Python quickly, we recommend Dive Into Python[13]. If that's not quite your style, there are many other books about Python[14].

[10] https://python.org/
[11] https://python.org/
[12] https://wiki.python.org/moin/BeginnersGuide/NonProgrammers
[13] https://www.diveinto.org/python3/
[14] https://wiki.python.org/moin/PythonBooks

CHAPTER

THREE

HOW-TO GUIDES

Here you'll find short answers to "How do I....?" types of questions. These how-to guides don't cover topics in depth – you'll find that material in the *Topics guides* (page 19) and the *Reference* (page 27). However, these guides will help you quickly accomplish common tasks using the "best practices".

3.1 How to create virtual environments for python with conda

In this section we will explain how to work with virtual environments using conda. A virtual environment is a named, isolated, working copy of Python that maintains its own files, directories, and paths so that you can work with specific versions of libraries or Python itself without affecting other Python projects. Virtual environments make it easy to cleanly separate different projects and avoid problems with different dependencies and version requirements across components. The conda command is the preferred interface for managing installations and virtual environments with the Anaconda Python distribution. If you have a vanilla Python installation or other Python distribution see virtualenv.

In the following we assume that the Anaconda Python distribution installed and accessible.

3.1.1 Check conda is installed and in your PATH.

Open a terminal client. Enter `conda -V` into the terminal command line and press enter. If conda is installed you should see somehting like the following.

```
$ conda -V
conda 4.6.8
```

3.1.2 Check conda is up to date.

In the terminal client enter

```
conda update conda
```

Update any packages if necessary by typing `y` to proceed.

3.1.3 Create a virtual environment for your project.

In the terminal client enter the following where yourenvname is the name you want to call your environment, and replace x.x with the Python version you wish to use. (To see a list of available python versions first, type `conda search "^python$"` and press enter.)

```
conda create -n yourenvname python=x.x anaconda
```

Press `y` to proceed. This will install the Python version and all the associated anaconda packaged libraries at path_to_your_anaconda_location/anaconda/envs/yourenvname

3.1.4 Activate your virtual environment.

To activate or switch into your virtual environment, simply type the following where yourenvname is the name you gave to your environement at creation.

```
conda activate yourenvname
```

Activating a conda environment modifies the PATH and shell variables to point to the specific isolated Python set-up you created. The command prompt will change to indicate which conda environemnt you are currently in by prepending (yourenvname). To see a list of all your environments, use the command `conda info -e`.

3.1.5 Install additional Python packages to a virtual environment.

To install additional packages only to your virtual environment, enter the following command where yourenvname is the name of your environemnt, and [package] is the name of the package you wish to install. Failure to specify `-n yourenvname` will install the package to the root Python installation.

```
conda install -n yourenvname [package]
```

3.1.6 Deactivate your virtual environment.

To end a session in the current environment, enter the following. There is no need to specify the envname - which ever is currently active will be deactivated, and the PATH and shell variables will be returned to normal.

```
conda deactivate
```

3.1.7 Delete a no longer needed virtual environment.

To delete a conda environment, enter the following, where yourenvname is the name of the environment you wish to delete.

```
conda remove -n yourenvname -all
```

3.1.8 Related info.

The offical conda documentation can be found here: https://conda.io/projects/conda/en/latest/user-guide/overview.html https://conda.io/projects/conda/en/latest/user-guide/getting-started.html.

3.2 Contributing

3.2.1 Contribute a patch

CHAPTER

FOUR

TOPICS GUIDES

This section explains and analyses some key concepts in numdifftools. It's less concerned with explaining *how to do things* than with helping you understand *how it works*.

4.1 Introduction derivative estimation

The general problem of differentiation of a function typically pops up in three ways in Python.

- The symbolic derivative of a function.
- Compute numerical derivatives of a function defined only by a sequence of data points.
- Compute numerical derivatives of a analytically supplied function.

Clearly the first member of this list is the domain of the symbolic toolbox SymPy, or some set of symbolic tools. Numerical differentiation of a function defined by data points can be achieved with the function gradient, or perhaps by differentiation of a curve fit to the data, perhaps to an interpolating spline or a least squares spline fit.

The third class of differentiation problems is where Numdifftools is valuable. This document will describe the methods used in Numdifftools and in particular the Derivative class.

4.2 Numerical differentiation of a general function of one variable

Surely you recall the traditional definition of a derivative, in terms of a limit.

$$f'(x) = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta} \tag{4.1}$$

For small δ, the limit approaches $f'(x)$. This is a one-sided approximation for the derivative. For a fixed value of δ, this is also known as a finite difference approximation (a forward difference.) Other approximations for the derivative are also available. We will see the origin of these approximations in the Taylor series expansion of a function $f(x)$ around some point x_0.

$$\begin{aligned} f(x_0+\delta) = f(x_0) + \delta f'(x_0) + \frac{\delta^2}{2} f''(x_0) + \frac{\delta^3}{6} f^{(3)}(x_0) + \\ \frac{\delta^4}{24} f^{(4)}(x_0) + \frac{\delta^5}{120} f^{(5)}(x_0) + \frac{\delta^6}{720} f^{(6)}(x_0) + ... \end{aligned} \tag{4.2}$$

Truncate the series in (4.2) to the first three terms, divide by δ and rearrange yields the forward difference approximation (4.1):

$$f'(x_0) = \frac{f(x_0+\delta) - f(x_0)}{\delta} - \frac{\delta}{2} f''(x_0) - \frac{\delta^2}{6} f'''(x_0) + ... \tag{4.3}$$

When δ is small, δ^2 and any higher powers are vanishingly small. So we tend to ignore those higher powers, and describe the approximation in (4.3) as a first order approximation since the error in this approximation approaches zero at the same rate as the first power of δ.[1] The values of $f''(x_0)$ and $f'''(x_0)$, while unknown to us, are fixed constants as δ varies.

Higher order approximations arise in the same fashion. The central difference (4.4) is a second order approximation.

$$f'(x_0) = \frac{f(x_0+\delta) - f(x_0-\delta)}{2\delta} - \frac{\delta^2}{3}f'''(x_0) + ... \tag{4.4}$$

4.3 Unequally spaced finite difference rules

While most finite difference rules used to differentiate a function will use equally spaced points, this fails to be appropriate when one does not know the final spacing. Adaptive quadrature rules can succeed by subdividing each sub-interval as necessary. But an adaptive differentiation scheme must work differently, since differentiation is a point estimate. Derivative generates a sequence of sample points that follow a log spacing away from the point in question, then it uses a single rule (generated on the fly) to estimate the desired derivative. Because the points are log spaced, the same rule applies at any scale, with only a scale factor applied.

4.4 Odd and even transformations of a function

Returning to the Taylor series expansion of $f(x)$ around some point x_0, an even function[2] around x_0 must have all the odd order derivatives vanish at x_0. An odd function has all its even derivatives vanish from its expansion. Consider the derived functions $f_{odd}(x)$ and $f_{even}(x)$.

$$f_{odd}(x) = \frac{f(x_0+x) - f(x_0-x)}{2} \tag{4.5}$$

$$f_{even}(x) = \frac{f(x_0+x) - 2f(x_0) + f(x_0-x)}{2} \tag{4.6}$$

The Taylor series expansion of $f_{odd}(x)$ around zero has the useful property that we have killed off any even order terms, but the odd order terms are identical to $f(x)$, as expanded around x_0.

$$f_{odd}(\delta) = \delta f'(x_0) + \frac{\delta^3}{6}f^{(3)}(x_0) + \frac{\delta^5}{120}f^{(5)}(x_0) + \frac{\delta^7}{5040}f^{(7)}(x_0) + ... \tag{4.7}$$

Likewise, the Taylor series expansion of $f_{even}(x)$ has no odd order terms or a constant term, but other even order terms that are identical to $f(x)$.

$$f_{even}(\delta) = \frac{\delta^2}{2}f^{(2)}(x_0) + \frac{\delta^4}{24}f^{(4)}(x_0) + \frac{\delta^6}{720}f^{(6)}(x_0) + \frac{\delta^8}{40320}f^{(8)}(x_0) + ... \tag{4.8}$$

The point of these transformations is we can rather simply generate a higher order approximation for any odd order derivatives of $f(x)$ by working with $f_{odd}(x)$. Even order derivatives of $f(x)$ are similarly generated from $f_{even}(x)$. For example, a second order approximation for $f'(x_0)$ is trivially written in (4.9) as a function of δ.

$$f'(x_0;\delta) = \frac{f_{odd}(\delta)}{\delta} - \frac{\delta^2}{6}f^{(3)}(x_0) \tag{4.9}$$

We can do better rather simply, so why not? (4.10) shows a fourth order approximation for $f'(x_0)$.

$$f'(x_0;\delta) = \frac{8f_{odd}(\delta) - f_{odd}(2\delta)}{6\delta} + \frac{\delta^4}{30}f^{(5)}(x_0) \tag{4.10}$$

[1] We would normally write these additional terms using O() notation, where all that matters is that the error term is $O(\delta)$ or perhaps $O(\delta^2)$, but explicit understanding of these error terms will be useful in the Richardson extrapolation step later on.

[2] An even function is one which expresses an even symmetry around a given point. An even symmetry has the property that $f(x) = f(-x)$. Likewise, an odd function expresses an odd symmetry, wherein $f(x) = -f(-x)$.

Again, the next non-zero term (4.11) in that expansion has a higher power of δ on it, so we would normally ignore it since the lowest order neglected term should dominate the behavior for small δ.

$$\frac{\delta^6}{252} f^{(7)}(x_0) \tag{4.11}$$

Derivative uses similar approximations for all derivatives of f up to any order. Of course, it is not always possible for evaluation of a function on both sides of a point, as central difference rules will require. In these cases, you can specify forward or backward difference rules as appropriate. You can also specify to use the complex step derivative, which we will outline in the next section.

4.5 Complex step derivative

The derivation of the complex-step derivative approximation is accomplished by replacing δ in (4.2) with a complex step ih:

$$f(x_0 + ih) = f(x_0) + ihf'(x_0) - \frac{h^2}{2} f''(x_0) - \frac{ih^3}{6} f^{(3)}(x_0) + \frac{h^4}{24} f^{(4)}(x_0) + \frac{ih^5}{120} f^{(5)}(x_0) - \frac{h^6}{720} f^{(6)}(x_0) - ... \tag{4.12}$$

Taking only the imaginary parts of both sides gives

$$\Im(f(x_0 + ih)) = hf'(x_0) - \frac{h^3}{6} f^{(3)}(x_0) + \frac{h^5}{120} f^{(5)}(x_0) - ... \tag{4.13}$$

Dividing with h and rearranging yields:

$$f'(x_0) = \Im(f(x_0 + ih))/h + \frac{h^2}{6} f^{(3)}(x_0) - \frac{h^4}{120} f^{(5)}(x_0) + ... \tag{4.14}$$

Terms with order h^2 or higher can safely be ignored since the interval h can be chosen up to machine precision without fear of rounding errors stemming from subtraction (since there are not any). Thus to within second-order the complex-step derivative approximation is given by:

$$f'(x_0) = \Im(f(x_0 + ih))/h \tag{4.15}$$

Next, consider replacing the step δ in (4.8) with the complex step $i^{\frac{1}{2}}h$:

$$f_{even}(i^{\frac{1}{2}}h) = \frac{ih^2}{2} f^{(2)}(x_0) - \frac{h^4}{24} f^{(4)}(x_0) - \frac{ih^6}{720} f^{(6)}(x_0) + \frac{h^8}{40320} f^{(8)}(x_0) + \frac{ih^{10}}{3628800} f^{(10)}(x_0) - ... \tag{4.16}$$

Similarly dividing with $h^2/2$ and taking only the imaginary components yields:

$$f^{(2)}(x_0) = \Im\left(2\, f_{even}(i^{\frac{1}{2}}h)\right)/h^2 + \frac{h^4}{360} f^{(6)}(x_0) - \frac{h^8}{1814400} f^{(10)}(x_0)... \tag{4.17}$$

This approximation is still subject to difference errors, but the error associated with this approximation is proportional to h^4. Neglecting these higher order terms yields:

$$f^{(2)}(x_0) = 2\Im\left(f_{even}(i^{\frac{1}{2}}h)\right)/h^2 = \Im(f(x_0 + i^{\frac{1}{2}}h) + f(x_0 - i^{\frac{1}{2}}h))/h^2 \tag{4.18}$$

See [**?**] and [**?**] for more details. The complex-step derivative in numdifftools.Derivative has truncation error $O(\delta^4)$ for both odd and even order derivatives for $n > 1$. For $n = 1$ the truncation error is on the order of $O(\delta^2)$, so truncation error can be eliminated by choosing steps to be very small. The first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, the function to differentiate needs to be analytic. This method does not work if it does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. For this reason the *central* method is the default method.

4.6 High order derivative

So how do we construct these higher order approximation formulas? Here we will deomonstrate the principle by computing the 6'th order central approximation for the first-order derivative. In order to do so we simply set $f_{odd}(\delta)$ equal to its 3-term Taylor expansion:

$$f_{odd}(\delta) = \sum_{i=0}^{2} \frac{\delta^{2i+1}}{(2i+1)!} f^{(2i+1)}(x_0) \tag{4.19}$$

By inserting three different stepsizes into (4.19), eg $\delta, \delta/2, \delta/4$, we get a set of linear equations:

$$\begin{bmatrix} 1 & \frac{1}{3!} & \frac{1}{5!} \\ \frac{1}{2} & \frac{1}{3!\,2^3} & \frac{1}{5!\,2^5} \\ \frac{1}{4} & \frac{1}{3!\,4^3} & \frac{1}{5!\,4^5} \end{bmatrix} \begin{bmatrix} \delta f'(x_0) \\ \delta^3 f^{(3)}(x_0) \\ \delta^5 f^{(5)}(x_0) \end{bmatrix} = \begin{bmatrix} f_{odd}(\delta) \\ f_{odd}(\delta/2) \\ f_{odd}(\delta/4) \end{bmatrix} \tag{4.20}$$

The solution of these equations are simply:

$$\begin{bmatrix} \delta f'(x_0) \\ \delta^3 f^{(3)}(x_0) \\ \delta^5 f^{(5)}(x_0) \end{bmatrix} = \frac{1}{3} \begin{bmatrix} \frac{1}{15} & \frac{-8}{3} & \frac{256}{15} \\ -8 & 272 & -512 \\ 512 & -5120 & 8192 \end{bmatrix} \begin{bmatrix} f_{odd}(\delta) \\ f_{odd}(\delta/2) \\ f_{odd}(\delta/4) \end{bmatrix} \tag{4.21}$$

The first row of (4.21) gives the coefficients for 6'th order approximation. Looking at at row two and three, we see also that this gives the 6'th order approximation for the 3'rd and 5'th order derivatives as bonus. Thus this is also a general method for obtaining high order differentiation rules. As previously noted these formulas have the additional benefit of beeing applicable to any scale, with only a scale factor applied.

4.7 Richardson extrapolation methodology applied to derivative estimation

Some individuals might suggest that the above set of approximations are entirely adequate for any sane person. Can we do better?

Suppose we were to generate several different estimates of the approximation in (4.3) for different values of δ at a fixed x_0. Thus, choose a single δ, estimate a corresponding resulting approximation to $f'(x_0)$, then do the same for $\delta/2$. If we assume that the error drops off linearly as $\delta \to 0$, then it is a simple matter to extrapolate this process to a zero step size. Our lack of knowledge of $f''(x_0)$ is irrelevant. All that matters is δ is small enough that the linear term dominates so we can ignore the quadratic term, therefore the error is purely linear.

$$f'(x_0) = \frac{f(x_0+\delta) - f(x_0)}{\delta} - \frac{\delta}{2} f''(x_0) \tag{4.22}$$

The linear extrapolant for this interval halving scheme as $\delta \to 0$ is given by:

$$f_0^{'} = 2f_{\delta/2}^{'} - f_{\delta}^{'} \tag{4.23}$$

Since I've always been a big fan of convincing myself that something will work before I proceed too far, lets try this out in Python. Consider the function e^x. Generate a pair of approximations to $f'(0)$, once at δ of 0.1, and the second approximation at $1/2$ that value. Recall that $\frac{d(e^x)}{dx} = e^x$, so at x = 0, the derivative should be exactly 1. How well will we do?

```
>>> from numpy import exp, allclose
>>> f = exp
>>> dx = 0.1
>>> df1 = (f(dx) - f(0))/dx
>>> allclose(df1, 1.05170918075648)
True
```

```
>>> df2 = (f(dx/2) - f(0))/(dx/2)
>>> allclose(df2, 1.02542192752048)
True
```

```
>>> allclose(2*df2 - df1, 0.999134674284488)
True
```

In fact, this worked very nicely, reducing the error to roughly 1 percent of our initial estimates. Should we be surprised at this reduction? Not if we recall that last term in (4.3). We saw there that the next term in the expansion was $O(\delta^2)$. Since δ was 0.1 in our experiment, that 1 percent number makes perfect sense.

The Richardson extrapolant in (4.23) assumed a linear process, with a specific reduction in δ by a factor of 2. Assume the two term (linear + quadratic) residual term in (4.3), evaluating our approximation there with a third value of δ. Again, assume the step size is cut in half again. The three term Richardson extrapolant is given by:

$$f'_0 = \frac{1}{3}f'_\delta - 2f'_{\delta/2} + \frac{8}{3}f'_{\delta/4} \tag{4.24}$$

A quick test in Python yields much better results yet.

```
>>> from numpy import exp, allclose
>>> f = exp
>>> dx = 0.1
```

```
>>> df1 = (f(dx) - f(0))/dx
>>> allclose(df1,  1.05170918075648)
True
```

```
>>> df2 = (f(dx/2) - f(0))/(dx/2)
>>> allclose(df2, 1.02542192752048)
True
```

```
>>> df3 = (f(dx/4) - f(0))/(dx/4)
>>> allclose(df3, 1.01260482097715)
True
```

```
>>> allclose(1./3*df1 - 2*df2 + 8./3*df3, 1.00000539448361)
True
```

Again, Derivative uses the appropriate multiple term Richardson extrapolants for all derivatives of f up to any order[3]. This, combined with the use of high order approximations for the derivatives, allows the use of quite large step sizes. See [**?**] and [**?**]. How to compute the multiple term Richardson extrapolants will be elaborated further in the next section.

4.8 Multiple term Richardson extrapolants

We shall now indicate how we can calculate the multiple term Richardson extrapolant for $f_{odd}(\delta)/\delta$ by rearranging (4.19):

$$\frac{f_{odd}(\delta)}{\delta} = f'(x_0) + \sum_{i=1}^{\infty} \frac{\delta^{2i}}{(2i+1)!} f^{(2i+1)}(x_0) \tag{4.25}$$

This equation has the form

$$\phi(\delta) = L + a_0\delta^2 + a_1\delta^4 + a_2\delta^6 + ... \tag{4.26}$$

[3] For practical purposes the maximum order of the derivative is between 4 and 10 depending on the function to differentiate and also the method used in the approximation.

where L stands for $f'(x_0)$ and $\phi(\delta)$ for the numerical differentiation formula $f_{odd}(\delta)/\delta$.

By neglecting higher order terms ($a_3\delta^8$) and inserting three different stepsizes into (4.26), eg $\delta, \delta/2, \delta/4$, we get a set of linear equations:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & \frac{1}{2^2} & \frac{1}{2^4} \\ 1 & \frac{1}{4^2} & \frac{1}{4^4} \end{bmatrix} \begin{bmatrix} L \\ \delta^2 a_0 \\ \delta^4 a_1 \end{bmatrix} = \begin{bmatrix} \phi(\delta) \\ \phi(\delta/2) \\ \phi(\delta/4) \end{bmatrix} \tag{4.27}$$

The solution of these equations are simply:

$$\begin{bmatrix} L \\ \delta^2 a_0 \\ \delta^4 a_1 \end{bmatrix} = \frac{1}{45} \begin{bmatrix} 1 & -20 & 64 \\ -20 & 340 & -320 \\ 64 & -320 & 256 \end{bmatrix} \begin{bmatrix} \phi(\delta) \\ \phi(\delta/2) \\ \phi(\delta/4) \end{bmatrix} \tag{4.28}$$

The first row of (4.28) gives the coefficients for Richardson extrapolation scheme.

4.9 Uncertainty estimates for Derivative

We can view the Richardson extrapolation step as a polynomial curve fit in the step size parameter δ. Our desired extrapolated value is seen as simply the constant term coefficient in that polynomial model. Remember though, this polynomial model (see (4.10) and (4.11)) has only a few terms in it with known non-zero coefficients. That is, we will expect a constant term a_0, a term of the form $a_1\delta^4$, and a third term $a_2\delta^6$.

A neat trick to compute the statistical uncertainty in the estimate of our desired derivative is to use statistical methodology for that error estimate. While I do appreciate that there is nothing truly statistical or stochastic in this estimate, the approach still works nicely, providing a very reasonable estimate in practice. A three term Richardson-like extrapolant, then evaluated at four distinct values for δ, will yield an estimate of the standard error of the constant term, with one spare degree of freedom. The uncertainty is then derived by multiplying that standard error by the appropriate percentile from the Students-t distribution.

```
>>> import scipy.stats as ss
>>> allclose(ss.t.cdf(12.7062047361747, 1), 0.975)
True
```

This critical level will yield a two-sided confidence interval of 95 percent.

These error estimates are also of value in a different sense. Since they are efficiently generated at all the different scales, the particular spacing which yields the minimum predicted error is chosen as the best derivative estimate. This has been shown to work consistently well. A spacing too large tends to have large errors of approximation due to the finite difference schemes used. But a too small spacing is bad also, in that we see a significant amplification of least significant fit errors in the approximation. A middle value generally seems to yield quite good results. For example, Derivative will estimate the derivative of e^x automatically. As we see, the final overall spacing used was 0.0078125.

```
>>> import numdifftools as nd
>>> from numpy import exp, allclose
>>> f = nd.Derivative(exp, full_output=True)
>>> val, info = f(1)
>>> allclose(val, 2.71828183)
True
>>> allclose(info.error_estimate, 6.927791673660977e-14)
True
>>> allclose(info.final_step, 0.0078125)
True
```

However, if we force the step size to be artificially large, then approximation error takes over.

```
>>> f = nd.Derivative(exp, step=1, full_output=True)
>>> val, info = f(1)
>>> allclose(val, 3.19452805)
True
>>> allclose(val-exp(1), 0.47624622)
True
>>> allclose(info.final_step, 1)
True
```

And if the step size is forced to be too small, then we see noise dominate the problem.

```
>>> f = nd.Derivative(exp, step=1e-10, full_output=True)
>>> val, info = f(1)
>>> allclose(val, 2.71828093)
True
>>> allclose(val - exp(1), -8.97648138e-07)
True
>>> allclose(info.final_step, 1.0000000e-10)
True
```

Numdifftools, like Goldilocks in the fairy tale bearing her name, stays comfortably in the middle ground.

CHAPTER

FIVE

REFERENCE

Technical reference material that details functions, modules, and objects included in numdifftools, describing what they are and what they do.

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5.1 Numdifftools summary

5.1.1 numdifftools.core module

Derivative (page 78)(fun[, step, method, order, n])	Calculate n-th derivative with finite difference approximation
Gradient (page 80)(fun[, step, method, order, n])	Calculate Gradient with finite difference approximation
Jacobian (page 88)(fun[, step, method, order, n])	Calculate Jacobian with finite difference approximation
Hessdiag (page 83)(f[, step, method, order])	Calculate Hessian diagonal with finite difference approximation
Hessian (page 85)(f[, step, method, order])	Calculate Hessian with finite difference approximation
directionaldiff (page 94)(f, x0, vec, **options)	Return directional derivative of a function of n variables

5.1.1.1 numdifftools.core.Derivative

class Derivative(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Calculate n-th derivative with finite difference approximation

Parameters

fun

[function] function of one array fun(x, **args*, ***kwds*)

step

[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in [‘complex’, ‘multicomplex’], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method

[{‘central’, ‘complex’, ‘multicomplex’, ‘forward’, ‘backward’}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

n
[int, optional] Order of the derivative.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

der
[ndarray] array of derivatives

See also:

Gradient **(page 80)**
Hessian **(page 85)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

1'st derivative of exp(x), at x == 1

```
>>> fd = nd.Derivative(np.exp)
>>> np.allclose(fd(1), 2.71828183)
True
```

```
>>> d2 = fd([1, 2])
>>> np.allclose(d2, [ 2.71828183,  7.3890561 ])
True
```

```
>>> def f(x):
...     return x**3 + x**2
```

```
>>> df = nd.Derivative(f)
>>> np.allclose(df(1), 5)
True
>>> ddf = nd.Derivative(f, n=2)
>>> np.allclose(ddf(1), 8)
True
```

Methods

__call__(x, *args, **kwds)	Call self as a function.

__init__(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Methods

__init__ (page 29)(fun[, step, method, order, n])	
set_richardson_rule (page 80)(step_ratio[, num_terms])	Set Richardson exptrapolation options

Attributes

method (page 80)	Defines the method used in the finite difference approximation.
method_order (page 80)	Defines the leading order of the error term in the Richardson extrapolation method.
n (page 80)	Order of the derivative.
order (page 80)	Defines the order of the error term in the Taylor approximation used.
step (page 80)	The step spacing(s) used in the approximation

5.1.1.2 numdifftools.core.Gradient

`class Gradient`(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Calculate Gradient with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

grad
[array] gradient

See also:

Derivative **(page 78),** *Hessian* **(page 85),** *Jacobian* **(page 88)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

If x0 is an n x m array, then fun is assumed to be a function of n * m variables.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

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Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> fun = lambda x: np.sum(x**2)
>>> dfun = nd.Gradient(fun)
>>> np.allclose(dfun([1,2,3]), [ 2.,  4.,  6.])
True
```

At [x,y] = [1,1], compute the numerical gradient # of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> x, y = 1, 1
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nd.Gradient(z)
>>> dz_dx, dz_dy = dz([x, y])
>>> np.allclose([dz_dx, dz_dy],
...             [ 3.7182818284590686, 1.7182818284590162])
True
```

At the global minimizer (1,1) of the Rosenbrock function, # compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> grad_rosen = nd.Gradient(rosen)
>>> df_dx, df_dy = grad_rosen([x, y])
>>> np.allclose([df_dx, df_dy], [0, 0])
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

__init__(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Methods

__init__ (page 31)(fun[, step, method, order, n])	
set_richardson_rule (page 83)(step_ratio[, num_terms])	Set Richardson exptrapolation options

Attributes

method (page 83)	Defines the method used in the finite difference approximation.
method_order (page 83)	Defines the leading order of the error term in the Richardson extrapolation method.
n (page 83)	Order of the derivative.
order (page 83)	Defines the order of the error term in the Taylor approximation used.
step (page 83)	The step spacing(s) used in the approximation

5.1.1.3 numdifftools.core.Jacobian

class Jacobian(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Calculate Jacobian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

jacob
[array] Jacobian

See also:

Derivative (page 78), *Hessian* (page 85), *Gradient* (page 80)

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

If fun returns a 1d array, it returns a Jacobian. If a 2d array is returned by fun (e.g., with a value for each observation), it returns a 3d array with the Jacobian of each observation with shape xk x nobs x xk. I.e., the Jacobian of the first observation would be [:, 0, :]

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape,  (10,))
True
```

```
>>> jfun = nd.Jacobian(fun)
>>> val = jfun([1, 2, 0.75])
>>> np.allclose(val, np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> jfun2 = nd.Jacobian(fun2)
>>> np.allclose(jfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
>>> jfun3 = nd.Jacobian(fun3)
```

```
>>> np.allclose(jfun3([1., 2., 3.]), [[[18.], [9.], [12.]], [[6.], [3.], [2.]]])
True
>>> np.allclose(jfun3([4., 5., 6.]), [[[180.], [144.], [240.]], [[30.], [24.],␣
↪[20.]]])
True
>>> np.allclose(jfun3(np.array([[1.,2.,3.]]).T), [[[18.], [9.], [12.]], [[6.],␣
↪[3.], [2.]]])
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

__init__(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Methods

__init__ (page 34)(fun[, step, method, order, n])	
set_richardson_rule (page 90)(step_ratio[, num_terms])	Set Richardson exptrapolation options

Attributes

method (page 90)	Defines the method used in the finite difference approximation.
method_order (page 90)	Defines the leading order of the error term in the Richardson extrapolation method.
n (page 90)	Order of the derivative.
order (page 90)	Defines the order of the error term in the Taylor approximation used.
step (page 90)	The step spacing(s) used in the approximation

5.1.1.4 numdifftools.core.Hessdiag

`class Hessdiag`(*f*, *step=None*, *method='central'*, *order=2*, ***options*)

Calculate Hessian diagonal with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximationorder : int, optional defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

hessdiag
[array] hessian diagonal

See also:

Derivative (page 78), *Hessian* (page 85), *Jacobian* (page 88), *Gradient* (page 80)

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> fun = lambda x : x[0] + x[1]**2 + x[2]**3
>>> Hfun = nd.Hessdiag(fun, full_output=True)
>>> hd, info = Hfun([1,2,3])
>>> np.allclose(hd, [0.,   2.,  18.])
True
```

```
>>> np.all(info.error_estimate < 1e-11)
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

`__init__`(*f*, *step=None*, *method='central'*, *order=2*, ***options*)

Methods

__init__ (page 36)(f[, step, method, order])	
set_richardson_rule (page 85)(step_ratio[, num_terms])	Set Richardson exptrapolation options

Attributes

method (page 85)	Defines the method used in the finite difference approximation.
method_order (page 85)	Defines the leading order of the error term in the Richardson extrapolation method.
n (page 85)	Order of the derivative.
order (page 85)	Defines the order of the error term in the Taylor approximation used.
step (page 85)	The step spacing(s) used in the approximation

5.1.1.5 numdifftools.core.Hessian

class Hessian(*f*, *step=None*, *method='central'*, *order=None*, ***options*)

Calculate Hessian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

hess
[ndarray] array of partial second derivatives, Hessian

See also:

Derivative **(page 78),** *Hessian* **(page 85)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Computes the Hessian according to method as: 'forward' (4.7), 'central' (4.9) and 'complex' (4.10):

$$((f(x + d_j e_j + d_k e_k) + f(x) - f(x + d_j e_j) - f(x + d_k e_k)))/(d_j d_k) \tag{5.1}$$

$$((f(x + d_j e_j + d_k e_k) - f(x + d_j e_j - d_k e_k)) - (f(x - d_j e_j + d_k e_k) - f(x - d_j e_j - d_k e_k))/(4 d_j d_k) \tag{5.2}$$

$$imag(f(x + i d_j e_j + d_k e_k) - f(x + i d_j e_j - d_k e_k))/(2 d_j d_k) \tag{5.3}$$

where e_j is a vector with element j is one and the rest are zero and d_j is a scalar spacing $steps_j$.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nd.Hessian(rosen)
>>> h = Hfun([1, 1])
>>> h
array([[ 842., -420.],
       [-420.,  210.]])
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nd.Hessian(fun)
>>> h2 = Hfun2([0, 0])
>>> h2
array([[-1.,  1.],
       [ 1., -1.]])
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

__init__(*f*, *step=None*, *method='central'*, *order=None*, ***options*)

Methods

__init__ (page 38)(f[, step, method, order])	
set_richardson_rule (page 87)(step_ratio[, num_terms])	Set Richardson exptrapolation options

Attributes

method (page 87)	Defines the method used in the finite difference approximation.
method_order (page 87)	Defines the leading order of the error term in the Richardson extrapolation method.
n (page 87)	Order of the derivative.
order (page 87)	Defines the order of the error term in the Taylor approximation used.
step (page 88)	The step spacing(s) used in the approximation

5.1.1.6 numdifftools.core.directionaldiff

directionaldiff(*f*, *x0*, *vec*, ***options*)

Return directional derivative of a function of n variables

Parameters

f: function
analytical function to differentiate.

x0: array
vector location at which to differentiate 'f'. If x0 is an nXm array, then 'f' is assumed to be a function of n*m variables.

vec: array
vector defining the line along which to take the derivative. It should be the same size as x0, but need not be a vector of unit length.

****options:**
optional arguments to pass on to Derivative.

Returns

dder: scalar
estimate of the first derivative of 'f' in the specified direction.

See also:

Derivative **(page 78)**
Gradient **(page 80)**

Examples

At the global minimizer (1,1) of the Rosenbrock function, compute the directional derivative in the direction [1 2]

```
>>> import numpy as np
>>> import numdifftools as nd
>>> vec = np.r_[1, 2]
>>> rosen = lambda x: (1-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> dd, info = nd.directionaldiff(rosen, [1, 1], vec, full_output=True)
>>> np.allclose(dd, 0)
True
>>> np.abs(info.error_estimate)<1e-14
True
```

5.1.2 Step generators

BasicMaxStepGenerator (page 131)(base_step, step_ratio, ...)	Generates a sequence of steps of decreasing magnitude
BasicMinStepGenerator (page 132)(base_step, step_ratio, ...)	Generates a sequence of steps of decreasing magnitude
MinStepGenerator (page 133)([base_step, step_ratio, ...])	Generates a sequence of steps
MaxStepGenerator (page 132)([base_step, step_ratio, ...])	Generates a sequence of steps

5.1.2.1 numdifftools.step_generators.BasicMaxStepGenerator

class BasicMaxStepGenerator(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Generates a sequence of steps of decreasing magnitude

where

steps = base_step * step_ratio ** (-i + offset)

for i=0, 1,.., num_steps-1.

Parameters

base_step
[float, array-like.] Defines the start step, i.e., maximum step

step_ratio
[real scalar.] Ratio between sequential steps generated. Note: Ratio > 1

num_steps
[scalar integer.] defines number of steps generated.

offset
[real scalar, optional, default 0] offset to the base step

Examples

```
>>> from numdifftools.step_generators import BasicMaxStepGenerator
>>> step_gen = BasicMaxStepGenerator(base_step=2.0, step_ratio=2,
...                                  num_steps=4)
>>> [s for s in step_gen()]
[2.0, 1.0, 0.5, 0.25]
```

__init__(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Methods

__init__ (page 40)(base_step, step_ratio, num_steps[, ...])	

5.1.2.2 numdifftools.step_generators.BasicMinStepGenerator

class BasicMinStepGenerator(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Generates a sequence of steps of decreasing magnitude

where

steps = base_step * step_ratio ** (i + offset), i=num_steps-1,... 1, 0.

Parameters

base_step
[float, array-like.] Defines the end step, i.e., minimum step

step_ratio
[real scalar.] Ratio between sequential steps generated. Note: Ratio > 1

num_steps
[scalar integer.] defines number of steps generated.

offset
[real scalar, optional, default 0] offset to the base step

Examples

```
>>> from numdifftools.step_generators import BasicMinStepGenerator
>>> step_gen = BasicMinStepGenerator(base_step=0.25, step_ratio=2,
...                                  num_steps=4)
>>> [s for s in step_gen()]
[2.0, 1.0, 0.5, 0.25]
```

__init__(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Methods

__init__	(page 41)(base_step, step_ratio, num_steps[, ...])

5.1.2.3 numdifftools.step_generators.MinStepGenerator

class MinStepGenerator(*base_step=None*, *step_ratio=None*, *num_steps=None*, *step_nom=None*, *offset=0*, *num_extrap=0*, *use_exact_steps=True*, *check_num_steps=True*, *scale=None*)

Generates a sequence of steps

where

steps = step_nom * base_step * step_ratio ** (i + offset)

for i = num_steps-1,... 1, 0.

Parameters

base_step
[float, array-like, optional] Defines the minimum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 2] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, optional] scale used in base step. If not None it will override the default computed with the default_scale function.

__init__(*base_step=None*, *step_ratio=None*, *num_steps=None*, *step_nom=None*, *offset=0*, *num_extrap=0*, *use_exact_steps=True*, *check_num_steps=True*, *scale=None*)

Methods

__init__ (page 42)([base_step, step_ratio, num_steps, ...])	
step_generator_function (page 134)(x[, method, n, order])	Step generator function

Attributes

base_step (page 134)	Base step defines the minimum or maximum step when offset==0.
min_num_steps (page 134)	Minimum number of steps required given the differentiation method and order.
num_steps (page 134)	Defines number of steps generated
scale (page 134)	Scale used in base step.
step_nom (page 134)	Nominal step
step_ratio (page 134)	Ratio between sequential steps generated

5.1.2.4 numdifftools.step_generators.MaxStepGenerator

class MaxStepGenerator(*base_step=2.0*, *step_ratio=None*, *num_steps=15*, *step_nom=None*, *offset=0*, *num_extrap=9*, *use_exact_steps=False*, *check_num_steps=True*, *scale=500*)

Generates a sequence of steps

where

steps = step_nom * base_step * step_ratio ** (-i + offset)

for i = 0, 1, ..., num_steps-1.

Parameters

base_step
[float, array-like, default 2.0] Defines the maximum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 2 or 1.6] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, default 500] scale used in base step.

__init__(*base_step=2.0*, *step_ratio=None*, *num_steps=15*, *step_nom=None*, *offset=0*, *num_extrap=9*, *use_exact_steps=False*, *check_num_steps=True*, *scale=500*)

Methods

__init__ (page 43)([base_step, step_ratio, num_steps, ...])	
step_generator_function(x[, method, n, order])	Step generator function

Attributes

base_step	Base step defines the minimum or maximum step when offset==0.
min_num_steps	Minimum number of steps required given the differentiation method and order.
num_steps	Defines number of steps generated
scale	Scale used in base step.
step_nom	Nominal step
step_ratio	Ratio between sequential steps generated

5.1.3 numdifftools.extrapolation module

convolve (page 97)(sequence, rule, **kwds)	Wrapper around scipy.ndimage.convolve1d that allows complex input.
Dea (page 95)([limexp])	Extrapolate a slowly convergent sequence using repeated Shanks transformations.
dea3 (page 97)(v_0, v_1, v_2[, symmetric])	Extrapolate a slowly convergent sequence using Shanks transformations.
Richardson (page 96)([step_ratio, step, order, num_terms])	Extrapolates a sequence with Richardsons method

5.1.3.1 numdifftools.extrapolation.convolve

convolve(*sequence*, *rule*, ***kwds*)

Wrapper around scipy.ndimage.convolve1d that allows complex input.

5.1.3.2 numdifftools.extrapolation.Dea

class Dea(*limexp=50*)

Extrapolate a slowly convergent sequence using repeated Shanks transformations.

Notes

DEA attempts to extrapolate nonlinearly by Shanks transformations to a better estimate of the sequence's limiting value, thus improving the rate of convergence. The epsilon algorithm of P. Wynn, see [1]_, is used to perform the non-linear Shanks transformations. The routine is a translation of the DQELG function found in the QUADPACK fortran library, see [2]_ and [3]_.

List of major variables:

LIMEXP: scalar integer
The maximum number of elements the epsilon table data can contain. The epsilon table is stored in the first (LIMEXP+2) entries of EPSTAB.

EPSTAB: real vector or size (LIMEXP+2+3)

The first LIMEXP+2 elements contains the two lower diagonals of the triangular epsilon table. The elements are numbered starting at the right-hand corner of the

triangle.

E0,E1,E2,E3: real scalars
The 4 elements on which the computation of a new element in the epsilon table is based.

NRES: scalar integer
Number of extrapolation results actually generated by the epsilon algorithm in prior calls to the routine.

NEWELM: scalar integer
Number of elements to be computed in the new diagonal of the epsilon table. The condensed epsilon table is computed. Only those elements needed for the computation of the next diagonal are preserved.

RES: real scalar
New element in the new diagonal of the epsilon table.

ERROR: real scalar
An estimate of the absolute error of RES. The routine decides whether RESULT=RES or RESULT=SVALUE by comparing ERROR with abserr from the previous call.

RES3LA: real vector of size 3
Contains at most the last 3 results.

__init__(*limexp=50*)

Methods

__init__ (page 45)([limexp])	

Attributes

limexp (page 96)	Maximum number of elements the epsilon table data.

5.1.3.3 numdifftools.extrapolation.dea3

dea3(*v_0*, *v_1*, *v_2*, *symmetric=False*)

Extrapolate a slowly convergent sequence using Shanks transformations.

Parameters

v_0, v_1, v_2
[array-like] 3 values of a convergent sequence to extrapolate

Returns

result
[array-like] extrapolated value

abserr
[array-like] absolute error estimate

See also:

Dea **(page 95)**

Notes

DEA3 attempts to extrapolate nonlinearly by Shanks transformations to a better estimate of the sequence's limiting value based on only three values. The epsilon algorithm of P. Wynn, see [Rc8bfc08f7c28-1], is used to perform the non-linear Shanks transformations. The routine is a vectorized translation of the DQELG function found in the QUADPACK fortran library for LIMEXP=3, see [Rc8bfc08f7c28-2] and [Rc8bfc08f7c28-3].

References

Examples

integrate sin(x) from 0 to pi/2

```
>>> import numpy as np
>>> import numdifftools as nd
>>> Ei= np.zeros(3)
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(3):
...     x = linfun(k)
...     Ei[k] = np.trapz(np.sin(x),x)
>>> [En, err] = nd.dea3(Ei[0], Ei[1], Ei[2])
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.allclose(En, 1)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
```

5.1.3.4 numdifftools.extrapolation.Richardson

class Richardson(*step_ratio=2.0*, *step=1*, *order=1*, *num_terms=2*)

Extrapolates a sequence with Richardsons method

Parameters

step_ratio: real scalar
Ratio between sequential steps, h, generated.

step: scalar integer
Defines the step between exponents in the error polynomial, i.e., step = k_1 - k_0 = k_2 - k_1 = ... = k_{i+1} - k_i

order: scalar integer
Leading order of truncation error.

num_terms: scalar integer
Number of terms used in the polynomial fit.

Notes

Suppose f(h) is an approximation of L (exact value) that depends on a positive step size h described with a sequence of the form

L = f(h) + a0 * h^k_0 + a1 * h^k_1+ a2 * h^k_2 + ...

where the ai are unknown constants and the k_i are known constants such that h^k_i > h^(k_i+1).

If we evaluate the right hand side for different stepsizes h we can fit a polynomial to that sequence of approximations. This is exactly what this class does. Here k_0 is the leading order step size behavior of truncation error as L = f(h)+O(h^k_0) (f(h) -> L as h -> 0, but f(0) != L) and k_i = order + step * i .

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> n = 3
>>> Ei = np.zeros((n,1))
>>> h = np.zeros((n,1))
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(n):
...     x = linfun(k)
...     h[k] = x[1]
...     Ei[k] = np.trapz(np.sin(x),x)
>>> En, err, step = nd.Richardson(step=1, order=1)(Ei, h)
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
>>> np.allclose(En, 1)
True
```

__init__(*step_ratio=2.0*, *step=1*, *order=1*, *num_terms=2*)

Methods

__init__ (page 47)([step_ratio, step, order, num_terms])	
extrapolate (page 97)(sequence, steps)	Extrapolate sequence
rule (page 97)([sequence_length])	Returns extrapolation rule.

5.1.4 numdifftools.limits module

CStepGenerator (page 110)([base_step, step_ratio, ...])	Generates a sequence of steps
Limit (page 111)(fun[, step, method, order, full_output])	Compute limit of a function at a given point
Residue (page 113)(f[, step, method, order, ...])	Compute residue of a function at a given point

5.1.4.1 numdifftools.limits.CStepGenerator

class CStepGenerator(*base_step=None*, *step_ratio=4.0*, *num_steps=None*, *step_nom=None*, *offset=0*, *scale=1.2*, ***options*)

Generates a sequence of steps

where

steps = base_step * step_nom * (exp(1j*dtheta) * step_ratio) ** (i + offset)

for i = 0, 1, ..., num_steps-1

Parameters

base_step
[float, array-like, default None] Defines the minimum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 4.0] Ratio between sequential steps generated.

num_steps
[scalar integer, optional,] defines number of steps generated. If None the value is 2 * int(round(16.0/log(abs(step_ratio)))) + 1

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

use_exact_steps
[boolean, default True.] If true make sure exact steps are generated.

scale
[real scalar, default 1.2] scale used in base step.

path
['radial' or 'spiral'] Specifies the type of path to take the limit along. Default 'radial'.

dtheta: real scalar, default pi/8
If the path is 'spiral' it will follow an exponential spiral into the limit, with angular steps at dtheta radians.

__init__(*base_step=None*, *step_ratio=4.0*, *num_steps=None*, *step_nom=None*, *offset=0*, *scale=1.2*, ***options*)

Methods

__init__ (page 48)([base_step, step_ratio, num_steps, ...])	
step_generator_function(x[, method, n, order])	Step generator function

Attributes

base_step	Base step defines the minimum or maximum step when offset==0.
dtheta (page 111)	Angular steps in radians used for the exponential spiral path.
min_num_steps	Minimum number of steps required given the differentiation method and order.
num_steps (page 111)	The number of steps generated
scale	Scale used in base step.
step_nom	Nominal step
step_ratio (page 111)	Ratio between sequential steps generated.

5.1.4.2 numdifftools.limits.Limit

class Limit(*fun*, *step=None*, *method='above'*, *order=4*, *full_output=False*, ***options*)

Compute limit of a function at a given point

Parameters

fun
[callable] function fun(z, **args*, ***kwds*) to compute the limit for z->z0. The function, fun, is assumed to return a result of the same shape and size as its input, *z*.

step: float, complex, array-like or StepGenerator object, optional
Defines the spacing used in the approximation. Default is CStepGenerator(base_step=step, **options)

method
[{'above', 'below'}] defines if the limit is taken from *above* or *below*

order: positive scalar integer, optional.
defines the order of approximation used to find the specified limit. The order must be member of [1 2 3 4 5 6 7 8]. 4 is a good compromise.

full_output: bool
If true return additional info.

options:
options to pass on to CStepGenerator

Returns

limit_fz: array like
estimated limit of f(z) as z –> z0

info:
Only given if full_output is True and contains the following:

error estimate: ndarray
95 % uncertainty estimate around the limit, such that abs(limit_fz - lim z->z0 f(z)) < error_estimate

final_step: ndarray
final step used in approximation

Notes

Limit computes the limit of a given function at a specified point, z0. When the function is evaluable at the point in question, this is a simple task. But when the function cannot be evaluated at that location due to a singularity, you may need a tool to compute the limit. *Limit* does this, as well as produce an uncertainty estimate in the final result.

The methods used by *Limit* are Richardson extrapolation in a combination with Wynn's epsilon algorithm which also yield an error estimate. The user can specify the method order, as well as the path into z0. z0 may be real or complex. *Limit* uses a proportionally cascaded series of function evaluations, moving away from your point of evaluation along a path along the real line (or in the complex plane for complex z0 or step.) The *step_ratio* is the ratio used between sequential steps. The sign of step allows you to specify a limit from above or below. Negative values of step will cause the limit to be taken approaching z0 from below.

A smaller *step_ratio* means that *Limit* will take more function evaluations to evaluate the limit, but the result will potentially be less accurate. The *step_ratio* MUST be a scalar larger than 1. A value in the range [2,100] is recommended. 4 seems a good compromise.

```
>>> import numpy as np
>>> from numdifftools.limits import Limit
>>> def f(x): return np.sin(x)/x
>>> lim_f0, err = Limit(f, full_output=True)(0)
>>> np.allclose(lim_f0, 1)
True
>>> np.allclose(err.error_estimate, 1.77249444610966e-15)
True
```

Compute the derivative of cos(x) at x == pi/2. It should be -1. The limit will be taken as a function of the differential parameter, dx.

```
>>> x0 = np.pi/2;
>>> def g(x): return (np.cos(x0+x)-np.cos(x0))/x
>>> lim_g0, err = Limit(g, full_output=True)(0)
>>> np.allclose(lim_g0, -1)
True
>>> err.error_estimate < 1e-14
True
```

Compute the residue at a first order pole at z = 0 The function 1./(1-exp(2*z)) has a pole at z == 0. The residue is given by the limit of z*fun(z) as z –> 0. Here, that residue should be -0.5.

```
>>> def h(z): return -z/(np.expm1(2*z))
>>> lim_h0, err = Limit(h, full_output=True)(0)
>>> np.allclose(lim_h0, -0.5)
True
>>> err.error_estimate < 1e-14
True
```

Compute the residue of function 1./sin(z)**2 at z = 0. This pole is of second order thus the residue is given by the limit of z**2*fun(z) as z –> 0.

```
>>> def g(z): return z**2/(np.sin(z)**2)
>>> lim_gpi, err = Limit(g, full_output=True)(0)
>>> np.allclose(lim_gpi, 1)
True
>>> err.error_estimate < 1e-14
True
```

A more difficult limit is one where there is significant subtractive cancellation at the limit point. In the following example, the cancellation is second order. The true limit should be 0.5.

```
>>> def k(x): return (x*np.exp(x)-np.expm1(x))/x**2
>>> lim_k0,err = Limit(k, full_output=True)(0)
>>> np.allclose(lim_k0, 0.5)
True
>>> err.error_estimate < 1.0e-8
True
```

```
>>> def h(x): return  (x-np.sin(x))/x**3
>>> lim_h0, err = Limit(h, full_output=True)(0)
>>> np.allclose(lim_h0, 1./6)
True
>>> err.error_estimate < 1e-8
True
```

__init__(*fun*, *step=None*, *method='above'*, *order=4*, *full_output=False*, ***options*)

Methods

__init__ (page 51)(fun[, step, method, order, full_output])	
limit (page 113)(x, *args, **kwds)	Return lim f(z) as z-> x

Attributes

step	The step spacing(s) used in the approximation

5.1.4.3 numdifftools.limits.Residue

class Residue(*f*, *step=None*, *method='above'*, *order=None*, *pole_order=1*, *full_output=False*, ***options*)

Compute residue of a function at a given point

Parameters

fun
: [callable] function fun(z, **args*, ***kwds*) to compute the Residue at z=z0. The function, fun, is assumed to return a result of the same shape and size as its input, *z*.

step: float, complex, array-like or StepGenerator object, optional
: Defines the spacing used in the approximation. Default is CStepGenerator(base_step=step, **options)

method
: [{'above', 'below'}] defines if the limit is taken from *above* or *below*

order: positive scalar integer, optional.
: defines the order of approximation used to find the specified limit. The order must be member of [1 2 3 4 5 6 7 8]. 4 is a good compromise.

pole_order
: [scalar integer] specifies the order of the pole at z0.

full_output: bool
: If true return additional info.

options:
: options to pass on to CStepGenerator

Returns

res_fz: array like
estimated residue, i.e., limit of f(z)*(z-z0)**pole_order as z –> z0 When the residue is estimated as approximately zero,

the wrong order pole may have been specified.

info: namedtuple,
Only given if full_output is True and contains the following:

error estimate: ndarray
95 % uncertainty estimate around the residue, such that abs(res_fz - lim z->z0 f(z)*(z-z0)**pole_order) < error_estimate Large uncertainties here suggest that the wrong order pole was specified for f(z0).

final_step: ndarray
final step used in approximation

Notes

Residue computes the residue of a given function at a simple first order pole, or at a second order pole.

The methods used by residue are polynomial extrapolants, which also yield an error estimate. The user can specify the method order, as well as the order of the pole.

z0 - scalar point at which to compute the residue. z0 may be
real or complex.

See the document DERIVEST.pdf for more explanation of the algorithms behind the parameters of Residue. In most cases, the user should never need to specify anything other than possibly the PoleOrder.

Examples

A first order pole at z = 0

```
>>> import numpy as np
>>> from numdifftools.limits import Residue
>>> def f(z): return -1./(np.expm1(2*z))
>>> res_f, info = Residue(f, full_output=True)(0)
>>> np.allclose(res_f, -0.5)
True
>>> info.error_estimate < 1e-14
True
```

A second order pole around z = 0 and z = pi >>> def h(z): return 1.0/np.sin(z)**2 >>> res_h, info = Residue(h, full_output=True, pole_order=2)([0, np.pi]) >>> np.allclose(res_h, 1) True >>> (info.error_estimate < 1e-10).all() True

__init__(*f*, *step=None*, *method='above'*, *order=None*, *pole_order=1*, *full_output=False*, ***options*)

Methods

__init__ (page 52)(f[, step, method, order, ...])	

limit(x, *args, **kwds)	Return lim f(z) as z-> x

Attributes

step	The step spacing(s) used in the approximation

5.1.5 numdifftools.multicomplex module

Bicomplex (page 115)(z1, z2)	Creates an instance of a Bicomplex object.

5.1.5.1 numdifftools.multicomplex.Bicomplex

class Bicomplex(*z1*, *z2*)

Creates an instance of a Bicomplex object. zeta = z1 + j*z2, where z1 and z2 are complex numbers.

__init__(*z1*, *z2*, *dtype=<class 'numpy.complex128'>*)

Methods

__init__ (page 53)(z1, z2[, dtype])	
arccos (page 115)()	
arccosh (page 115)()	
arcsin (page 115)()	
arcsinh (page 115)()	
arctan (page 115)()	
arctanh (page 115)()	
arg_c (page 115)()	
arg_c1p (page 115)()	
asarray (page 115)(other)	
conjugate (page 115)()	
cos (page 115)()	
cosh (page 115)()	

continues on next page

Table 5.1 – continued from previous page

cot (page 115)()	
coth (page 115)()	
csc (page 115)()	
csch (page 115)()	
dot (page 115)(other)	
exp (page 115)()	
exp2 (page 115)()	
expm1 (page 115)()	
flat (page 115)(index)	
log (page 116)()	
log10 (page 116)()	
log1p (page 116)()	
log2 (page 116)()	
logaddexp (page 116)(other)	
logaddexp2 (page 116)(other)	
mat2bicomp (page 116)(arr)	
mod_c (page 116)()	Complex modulus
norm (page 116)()	
sec (page 116)()	
sech (page 116)()	
sin (page 116)()	
sinh (page 116)()	
sqrt (page 116)()	
tan (page 116)()	
tanh (page 116)()	

Attributes

z1 (page 116)
z2 (page 116)
imag (page 115)
imag1 (page 115)
imag12 (page 115)
imag2 (page 116)
real (page 116)
shape (page 116)
size (page 116)

5.1.6 numdifftools.nd_algopy module

Derivative (page 117)(fun[, n, method, full_output])	Calculate n-th derivative with Algorithmic Differentiation method
Gradient (page 118)(fun[, n, method, full_output])	Calculate Gradient with Algorithmic Differentiation method
Jacobian (page 123)(fun[, n, method, full_output])	Calculate Jacobian with Algorithmic Differentiation method
Hessdiag (page 120)(f[, method, full_output])	Calculate Hessian diagonal with Algorithmic Differentiation method
Hessian (page 121)(f[, method, full_output])	Calculate Hessian with Algorithmic Differentiation method
directionaldiff (page 125)(f, x0, vec, **options)	Return directional derivative of a function of n variables

5.1.6.1 numdifftools.nd_algopy.Derivative

class Derivative(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Calculate n-th derivative with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

n: int, optional
Order of the derivative.

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

der: ndarray
array of derivatives

See also:

Gradient **(page 118)**
Hessdiag **(page 120)**
Hessian **(page 121)**
Jacobian **(page 123)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

1'st and 2'nd derivative of exp(x), at x == 1

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> fd = nda.Derivative(np.exp)               # 1'st derivative
>>> np.allclose(fd(1), 2.718281828459045)
True
>>> fd5 = nda.Derivative(np.exp, n=5)          # 5'th derivative
>>> np.allclose(fd5(1), 2.718281828459045)
True
```

1'st derivative of x^3+x^4, at x = [0,1]

```
>>> fun = lambda x: x**3 + x**4
>>> fd3 = nda.Derivative(fun)
>>> np.allclose(fd3([0,1]), [ 0.,  7.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

__init__(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Methods

__init__ (page 56)(fun[, n, method, full_output])
computational_graph(x, *args, **kwds)

Attributes

fun

5.1.6.2 numdifftools.nd_algopy.Gradient

class Gradient(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Calculate Gradient with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

grad: array
gradient

See also:

Derivative **(page 117)**
Jacobian **(page 123)**
Hessdiag **(page 120)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> fun = lambda x: np.sum(x**2)
>>> df = nda.Gradient(fun, method='reverse')
>>> np.allclose(df([1,2,3]), [ 2.,  4.,  6.])
True
```

#At [x,y] = [1,1], compute the numerical gradient #of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nda.Gradient(z)
>>> grad2 = dz([1, 1])
>>> np.allclose(grad2, [ 3.71828183,  1.71828183])
True
```

#At the global minimizer (1,1) of the Rosenbrock function, #compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> rd = nda.Gradient(rosen)
>>> grad3 = rd([1,1])
>>> np.allclose(grad3, [ 0.,  0.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

__init__(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Methods

__init__ (page 58)(fun[, n, method, full_output])
computational_graph(x, *args, **kwds)

Attributes

fun

5.1.6.3 numdifftools.nd_algopy.Jacobian

class Jacobian(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Calculate Jacobian with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

jacob: array
Jacobian

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Hessdiag **(page 120)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
```

Jfun = nda.Jacobian(fun) # Todo: This does not work Jfun([1,2,0.75]).T # should be numerically zero array([[0., 0., 0., 0., 0., 0., 0., 0., 0., 0.],

[0., 0., 0., 0., 0., 0., 0., 0., 0., 0.], [0., 0., 0., 0., 0., 0., 0., 0., 0., 0.]])

```
>>> Jfun2 = nda.Jacobian(fun, method='reverse')
>>> res = Jfun2([1,2,0.75]).T # should be numerically zero
>>> np.allclose(res,
...                [[ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.],
...                 [ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.],
...                 [ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.]])
True
```

```
>>> f2 = lambda x : x[0]*x[1]*x[2]**2
>>> Jfun2 = nda.Jacobian(f2)
>>> np.allclose(Jfun2([1., 2., 3.]), [[ 18., 9., 12.]])
True
```

```
>>> Jfun21 = nda.Jacobian(f2, method='reverse')
>>> np.allclose(Jfun21([1., 2., 3.]), [[ 18., 9., 12.]])
True
```

```
>>> def fun3(x):
...     n = int(np.prod(np.shape(x[0])))
...     out = nda.algopy.zeros((2, n), dtype=x)
...     out[0] = x[0]*x[1]*x[2]**2
...     out[1] = x[0]*x[1]*x[2]
...     return out
>>> Jfun3 = nda.Jacobian(fun3)
```

```
>>> np.allclose(Jfun3([1., 2., 3.]), [[[18., 9., 12.]], [[6., 3., 2.]]])
True
>>> np.allclose(Jfun3([4., 5., 6.]), [[[180., 144., 240.]],
...                                   [[30., 24., 20.]]])
True
>>> np.allclose(Jfun3(np.array([[1.,2.,3.], [4., 5., 6.]]).T),
...              [[[18.,    0.,    9.,    0.,   12.,    0.],
...                [0.,  180.,    0.,  144.,    0.,  240.]],
...               [[6.,    0.,    3.,    0.,    2.,    0.],
...                [0.,   30.,    0.,   24.,    0.,   20.]]])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

__init__(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Methods

__init__ (page 61)(fun[, n, method, full_output])
computational_graph(x, *args, **kwds)

Attributes

fun

5.1.6.4 numdifftools.nd_algopy.Hessdiag

class Hessdiag(*f*, *method='forward'*, *full_output=False*)

Calculate Hessian diagonal with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

hessdiag
[ndarray] Hessian diagonal array of partial second order derivatives.

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Jacobian **(page 123)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nda.Hessdiag(rosen)
>>> h = Hfun([1, 1]) #  h =[ 842, 210]
>>> np.allclose(h, [ 842.,  210.])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nda.Hessdiag(fun)
>>> h2 = Hfun2([0, 0]) # h2 = [-1, -1]
>>> np.allclose(h2, [-1., -1.])
True
```

```
>>> Hfun3 = nda.Hessdiag(fun, method='reverse')
>>> h3 = Hfun3([0, 0]) # h2 = [-1, -1];
>>> np.allclose(h3, [-1., -1.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

__init__(*f*, *method='forward'*, *full_output=False*)

Methods

__init__ (page 62)(f[, method, full_output])
computational_graph(x, *args, **kwds)

Attributes

fun

5.1.6.5 numdifftools.nd_algopy.Hessian

class Hessian(*f*, *method='forward'*, *full_output=False*)

Calculate Hessian with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

hess
[ndarray] array of partial second derivatives, Hessian

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Jacobian **(page 123)**
Hessdiag **(page 120)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hf = nda.Hessian(rosen)
>>> h = Hf([1, 1]) #  h =[ 842 -420; -420, 210];
>>> np.allclose(h, [[ 842., -420.],
...                 [-420.,  210.]])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nda.Hessian(fun)
>>> h2 = Hfun2([0, 0]) # h2 = [-1 1; 1 -1]
>>> np.allclose(h2, [[-1.,  1.],
...                  [ 1., -1.]])
True
```

```
>>> Hfun3 = nda.Hessian(fun, method='reverse')
>>> h3 = Hfun3([0, 0]) # h2 = [-1, 1; 1, -1];
>>> np.allclose(h3, [[-1.,  1.],
...                  [ 1., -1.]])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

__init__(*f*, *method='forward'*, *full_output=False*)

Methods

__init__ (page 64)(f[, method, full_output])
computational_graph(x, *args, **kwds)

Attributes

fun

5.1.6.6 numdifftools.nd_algopy.directionaldiff

directionaldiff(*f*, *x0*, *vec*, ***options*)

Return directional derivative of a function of n variables

Parameters

fun: callable
analytical function to differentiate.

x0: array
vector location at which to differentiate fun. If x0 is an nxm array, then fun is assumed to be a function of n*m variables.

vec: array
vector defining the line along which to take the derivative. It should be the same size as x0, but need not be a vector of unit length.

****options:**
optional arguments to pass on to Derivative.

Returns

dder: scalar
estimate of the first derivative of fun in the specified direction.

See also:

Derivative **(page 117)**
Gradient **(page 118)**

Examples

At the global minimizer (1,1) of the Rosenbrock function, compute the directional derivative in the direction [1 2]

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> vec = np.r_[1, 2]
>>> rosen = lambda x: (1-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> dd = nda.directionaldiff(rosen, [1, 1], vec)
>>> np.allclose(dd, 0)
True
```

5.1.7 numdifftools.nd_scipy module

Gradient (page 126)(fun[, step, method, order, bounds, ...])	Calculate Gradient with finite difference approximation
Jacobian (page 126)(fun[, step, method, order, bounds, ...])	Calculate Jacobian with finite difference approximation

5.1.7.1 numdifftools.nd_scipy.Gradient

class Gradient(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Calculate Gradient with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
[{'central', 'complex', 'forward'}] defines the method used in the approximation.

See also:

Hessian, *Jacobian* (page 126)

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_scipy as nd
>>> fun = lambda x: np.sum(x**2)
>>> dfun = nd.Gradient(fun)
>>> np.allclose(dfun([1,2,3]), [ 2.,  4.,  6.])
True
```

At [x,y] = [1,1], compute the numerical gradient # of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nd.Gradient(z)
>>> grad2 = dz([1, 1])
>>> np.allclose(grad2, [ 3.71828183,  1.71828183])
True
```

At the global minimizer (1,1) of the Rosenbrock function, # compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> rd = nd.Gradient(rosen)
>>> grad3 = rd([1,1])
>>> np.allclose(grad3,[0, 0], atol=1e-7)
True
```

__init__(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Methods

__init__ (page 66)(fun[, step, method, order, bounds, ...])	

5.1.7.2 numdifftools.nd_scipy.Jacobian

class Jacobian(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Calculate Jacobian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
[{'central', 'complex', 'forward'}] defines the method used in the approximation.

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_scipy as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape, (10,))
True
>>> dfun = nd.Jacobian(fun)
>>> np.allclose(dfun([1, 2, 0.75]), np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> dfun2 = nd.Jacobian(fun2)
>>> np.allclose(dfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
```

TODO: The following does not work: der3 = nd.Jacobian(fun3)([1., 2., 3.]) np.allclose(der3, … [[18., 9., 12.], [6., 3., 2.]]) True np.allclose(nd.Jacobian(fun3)([4., 5., 6.]), … [[180., 144., 240.], [30., 24., 20.]]) True

np.allclose(nd.Jacobian(fun3)(np.array([[1.,2.,3.], [4., 5., 6.]]).T), … [[[18., 180.], … [9., 144.], … [12., 240.]], … [[6., 30.], … [3., 24.], … [2., 20.]]]) True

__init__(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Methods

__init__ (page 67)(fun[, step, method, order, bounds, ...])	

5.1.8 numdifftools.nd_statsmodels module

Hessian (page 128)(fun[, step, method, order])	Calculate Hessian with finite difference approximation
Jacobian (page 129)(fun[, step, method, order])	Calculate Jacobian with finite difference approximation

5.1.8.1 numdifftools.nd_statsmodels.Hessian

class Hessian(*fun*, *step=None*, *method='central'*, *order=None*)

Calculate Hessian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS**(1/3) for method==`forward`, *complex* or *central2* x * _EPS**(1/4) for method==`central`.

method
[{'central', 'complex', 'forward', 'backward'}] defines the method used in the approximation.

See also:

Jacobian **(page 129),** *Gradient* **(page 127)**

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_statsmodels as nd
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nd.Hessian(rosen)
>>> h = Hfun([1, 1])
>>> np.allclose(h, [[ 842., -420.], [-420.,  210.]])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nd.Hessian(fun)
>>> h2 = Hfun2([0, 0])
>>> np.allclose(h2, [[-1.,  1.], [ 1., -1.]])
True
```

__init__(*fun*, *step=None*, *method='central'*, *order=None*)

Methods

__init__ (page 68)(fun[, step, method, order])

Attributes

method
n (page 129)
order

5.1.8.2 numdifftools.nd_statsmodels.Jacobian

class Jacobian(*fun*, *step=None*, *method='central'*, *order=None*)

Calculate Jacobian with finite difference approximation

Parameters

fun
: [function] function of one array fun(x, **args*, ***kwds*)

step
: [float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
: [{'central', 'complex', 'forward', 'backward'}] defines the method used in the approximation.

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_statsmodels as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape, (10,))
True
>>> dfun = nd.Jacobian(fun)
>>> np.allclose(dfun([1, 2, 0.75]), np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> dfun2 = nd.Jacobian(fun2)
>>> np.allclose(dfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
>>> np.allclose(nd.Jacobian(fun3)([1., 2., 3.]), [[[18.], [9.], [12.]], [[6.],␣
↪[3.], [2.]]])
True
>>> np.allclose(nd.Jacobian(fun3)([4., 5., 6.]),
...             [[[180.], [144.], [240.]], [[30.], [24.], [20.]]])
True
```

```
>>> np.allclose(nd.Jacobian(fun3)(np.array([[1.,2.,3.], [4., 5., 6.]]).T),
...             [[[  18.,  180.],
...               [   9.,  144.],
...               [  12.,  240.]],
...              [[   6.,   30.],
...               [   3.,   24.],
...               [   2.,   20.]]])
True
```

__init__(*fun*, *step=None*, *method='central'*, *order=None*)

Methods

__init__ (page 70)(fun[, step, method, order])

Attributes

method
n
order

5.2 Numdifftools package details

5.2.1 numdifftools.tests package

5.2.1.1 numdifftools.tests.hamiltonian module

Created on Jun 25, 2016

@author: pab

class ClassicalHamiltonian

Bases: object[15]

Hamiltonian

Parameters

n

[scalar] number of ions in the chain

w
[scalar] angular trap frequency

C
[scalar] Coulomb constant times the electronic charge in SI units.

m
[scalar] the mass of a single trapped ion in the chain

`initialposition()`
Defines initial position as an estimate for the minimize process.

`normal_modes(eigenvalues)`
Return normal modes

Computed eigenvalues of the matrix Vx are of the form
(normal_modes)**2*m.

`potential(positionvector)`
Return potential

Parameters

positionvector: 1-d array (vector) of length n
positions of the n ions

`run_hamiltonian(hessian, verbose=True)`

5.2.1.2 numdifftools.tests.test_extrapolation module

`class TestExtrapolation`
Bases: `object`[16]

`setup_method()`

`test_dea3_on_trapz_sin()`

`test_dea_on_trapz_sin()`

`test_epsal()`

`test_richardson()`

`class TestRichardson`
Bases: `object`[17]

`setup_method()`

`test_order_step_combinations()`

[15] https://docs.python.org/3.7/library/functions.html#object
[16] https://docs.python.org/3.7/library/functions.html#object
[17] https://docs.python.org/3.7/library/functions.html#object

5.2.1.3 numdifftools.tests.test_fornberg module

class ExampleFunctions

Bases: object[18]

static fun0(*z*)

static fun1(*z*)

static fun10(*z*)

static fun11(*z*)

static fun12(*z*)

static fun13(*z*)

static fun14(*z*)

static fun2(*z*)

static fun3(*z*)

static fun4(*z*)

static fun5(*z*)

static fun6(*z*)

static fun7(*z*)

static fun8(*z*)

static fun9(*z*)

test_all_weights()

test_fd_derivative()

test_high_order_derivative() → None[19]

test_low_order_derivative_on_example_functions()

test_weights()

5.2.1.4 numdifftools.tests.test_limits module

Created on 28. aug. 2015

@author: pab

class TestCStepGenerator

Bases: object[20]

static test_default_base_step()

static test_default_generator()

static test_fixed_base_step()

[18] https://docs.python.org/3.7/library/functions.html#object
[19] https://docs.python.org/3.7/library/constants.html#None
[20] https://docs.python.org/3.7/library/functions.html#object

class TestLimit

Bases: object[21]

test_derivative_of_cos()

test_difficult_limit()

test_residue_1_div_1_minus_exp_x()

test_sinx_div_x()

class TestResidue

Bases: object[22]

test_residue_1_div_1_minus_exp_x()

test_residue_1_div_sin_x2()

5.2.1.5 numdifftools.tests.test_multicomplex module

Created on 22. apr. 2015

@author: pab

class TestBicomplex

Bases: object[23]

static test_add()

static test_arccos()

static test_arcsin()

static test_arg_c()

static test_assign()

test_conjugate()

static test_cos()

static test_der_abs()

static test_der_arccos()

static test_der_arccosh()

static test_der_arctan()

static test_der_cos()

static test_der_log()

static test_division()

static test_dot()

static test_eq()

test_flat()

[21] https://docs.python.org/3.7/library/functions.html#object
[22] https://docs.python.org/3.7/library/functions.html#object

static test_ge()

static test_gt()

test_init()

static test_le()

static test_lt()

static test_mod_c()

static test_multiplication()

test_neg()

test_norm()

static test_pow()

test_rdivision()

Test issue # 39

test_repr()

static test_rpow()

static test_rsub()

test_shape()

static test_sub()

static test_subsref()

class TestDerivative

Bases: object[24]

static test_all_first_derivatives()

static test_all_second_derivatives()

5.2.1.6 numdifftools.tests.test_nd_algopy module

class TestDerivative

Bases: object[25]

static test_derivative_cube()

Test for Issue 7

static test_derivative_exp() → None[26]

static test_derivative_on_log() → None[27]

test_derivative_on_sinh() → None[28]

static test_derivative_sin()

static test_directional_diff()

[23] https://docs.python.org/3.7/library/functions.html#object
[24] https://docs.python.org/3.7/library/functions.html#object

static test_fun_with_additional_parameters()

Test for issue #9

static test_high_order_derivative_cos()

class TestGradient

Bases: object[29]

static test_on_scalar_function()

class TestHessdiag

Bases: object[30]

static test_forward()

static test_reverse()

class TestHessian

Bases: object[31]

static test_hessian_cos_x_y__at_0_0()

test_run_hamiltonian()

class TestJacobian

Bases: object[32]

static test_issue_25()

static test_on_matrix_valued_function()

static test_on_scalar_function()

test_on_vector_valued_function()

static test_scalar_to_vector() → None[33]

5.2.1.7 numdifftools.tests.test_nd_scipy module

class TestGradient

Bases: object[34]

static test_on_scalar_function()

class TestJacobian

Bases: object[35]

test_issue_25()

test_on_matrix_valued_function()

static test_on_scalar_function()

[25] https://docs.python.org/3.7/library/functions.html#object
[26] https://docs.python.org/3.7/library/constants.html#None
[27] https://docs.python.org/3.7/library/constants.html#None
[28] https://docs.python.org/3.7/library/constants.html#None
[29] https://docs.python.org/3.7/library/functions.html#object
[30] https://docs.python.org/3.7/library/functions.html#object
[31] https://docs.python.org/3.7/library/functions.html#object
[32] https://docs.python.org/3.7/library/functions.html#object
[33] https://docs.python.org/3.7/library/constants.html#None
[34] https://docs.python.org/3.7/library/functions.html#object

test_on_vector_valued_function()

static test_scalar_to_vector() → None[36]

5.2.1.8 numdifftools.tests.test_numdifftools module

Test functions for numdifftools module

class TestDerivative

Bases: object[37]

test_backward_derivative_on_sinh()

test_central_and_forward_derivative_on_log()

static test_default_scale()

static test_derivative_cube()

Test for Issue 7

static test_derivative_exp()

static test_derivative_of_cos_x() → None[38]

static test_derivative_sin()

static test_derivative_with_step_options()

static test_directional_diff()

static test_fun_with_additional_parameters()

Test for issue #9

static test_high_order_derivative_cos()

test_infinite_functions()

class TestGradient

Bases: object[39]

static test_directional_diff()

static test_gradient()

static test_gradient_fulloutput()

Fix issue#52:

Gradient tries to apply squeeze to the output tuple containing both the result and the full_output object.

static test_issue_39()

Test that checks float/Bicomplex works

class TestHessdiag

Bases: object[40]

test_complex()

test_default_step()

[35] https://docs.python.org/3.7/library/functions.html#object
[36] https://docs.python.org/3.7/library/constants.html#None
[37] https://docs.python.org/3.7/library/functions.html#object
[38] https://docs.python.org/3.7/library/constants.html#None
[39] https://docs.python.org/3.7/library/functions.html#object

test_fixed_step() → None[41]

class TestHessian

Bases: object[42]

test_complex_hessian_issue_35()

static test_hessian_cos_x_y_at_0_0()

test_run_hamiltonian()

class TestJacobian

Bases: object[43]

static test_issue_25()

static test_issue_27a()

Test for memory-error

static test_issue_27b()

Test for memory-error

static test_jacobian_fulloutput()

test

static test_on_matrix_valued_function()

static test_on_scalar_function()

static test_on_vector_valued_function()

static test_scalar_to_vector() → None[44]

class TestRichardson

Bases: object[45]

static test_central_forward_backward()

static test_complex()

5.2.1.9 numdifftools.tests.test_scripts module

test__find_default_scale_run_all_benchmarks()

test_profile_numdifftools_main()

test_profile_numdifftools_profile_hessian()

test_run_gradient_and_hessian_benchmarks()

[40] https://docs.python.org/3.7/library/functions.html#object
[41] https://docs.python.org/3.7/library/constants.html#None
[42] https://docs.python.org/3.7/library/functions.html#object
[43] https://docs.python.org/3.7/library/functions.html#object
[44] https://docs.python.org/3.7/library/constants.html#None
[45] https://docs.python.org/3.7/library/functions.html#object

5.2.1.10 numdifftools.tests.test_step_generators module

`test__min_step_generator_with_step_nom1()`

`test_default_max_step_generator()`

`test_max_step_generator_default_base_step()`

`test_max_step_generator_with_base_step01()`

`test_min_step_generator_default_base_step()`

`test_min_step_generator_with_base_step01()`

`test_min_step_generator_with_step_ratio4()`

5.2.2 numdifftools.core module

numerical differentiation functions:

Derivative, Gradient, Jacobian, and Hessian

Author: Per A. Brodtkorb Created: 01.08.2008 Copyright: (c) pab 2008 Licence: New BSD

`class Derivative(`*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*`)`

Bases: `_Limit`

Calculate n-th derivative with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

n
[int, optional] Order of the derivative.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

der
[ndarray] array of derivatives

See also:

Gradient **(page 80)**
Hessian **(page 85)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

1'st derivative of exp(x), at x == 1

```
>>> fd = nd.Derivative(np.exp)
>>> np.allclose(fd(1), 2.71828183)
True
```

```
>>> d2 = fd([1, 2])
>>> np.allclose(d2, [ 2.71828183,  7.3890561 ])
True
```

```
>>> def f(x):
...     return x**3 + x**2
```

```
>>> df = nd.Derivative(f)
>>> np.allclose(df(1), 5)
True
>>> ddf = nd.Derivative(f, n=2)
>>> np.allclose(ddf(1), 8)
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

class info(*f_value*, *error_estimate*, *final_step*, *index*)

Bases: `tuple`[46]

count(*value*, */*)

Return number of occurrences of value.

property error_estimate

Alias for field number 1

property f_value

Alias for field number 0

property final_step

Alias for field number 2

property index

Alias for field number 3

property method

Defines the method used in the finite difference approximation.

property method_order

Defines the leading order of the error term in the Richardson extrapolation method.

property n

Order of the derivative.

property order

Defines the order of the error term in the Taylor approximation used.

set_richardson_rule(*step_ratio*, *num_terms=2*)

Set Richardson exptrapolation options

property step

The step spacing(s) used in the approximation

class Gradient(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Bases: *Jacobian* (page 88)

Calculate Gradient with finite difference approximation

Parameters

fun

[function] function of one array fun(x, **args*, ***kwds*)

[46] https://docs.python.org/3.7/library/stdtypes.html#tuple

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

grad
[array] gradient

See also:

Derivative **(page 78),** *Hessian* **(page 85),** *Jacobian* **(page 88)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

If x0 is an n x m array, then fun is assumed to be a function of n * m variables.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> fun = lambda x: np.sum(x**2)
>>> dfun = nd.Gradient(fun)
>>> np.allclose(dfun([1,2,3]), [ 2.,  4.,  6.])
True
```

At [x,y] = [1,1], compute the numerical gradient # of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> x, y = 1, 1
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nd.Gradient(z)
>>> dz_dx, dz_dy = dz([x, y])
>>> np.allclose([dz_dx, dz_dy],
...             [ 3.7182818284590686, 1.7182818284590162])
True
```

At the global minimizer (1,1) of the Rosenbrock function, # compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> grad_rosen = nd.Gradient(rosen)
>>> df_dx, df_dy = grad_rosen([x, y])
>>> np.allclose([df_dx, df_dy], [0, 0])
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

class info(*f_value*, *error_estimate*, *final_step*, *index*)

Bases: `tuple`[47]

count(*value*, */*)

Return number of occurrences of value.

property error_estimate

Alias for field number 1

property f_value

Alias for field number 0

property final_step

Alias for field number 2

property index

Alias for field number 3

property method

Defines the method used in the finite difference approximation.

property method_order

Defines the leading order of the error term in the Richardson extrapolation method.

property n

Order of the derivative.

property order

Defines the order of the error term in the Taylor approximation used.

set_richardson_rule(*step_ratio*, *num_terms=2*)

Set Richardson exptrapolation options

property step

The step spacing(s) used in the approximation

class Hessdiag(*f*, *step=None*, *method='central'*, *order=2*, ***options*)

Bases: *Derivative* (page 78)

Calculate Hessian diagonal with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in [‘complex’, ‘multicomplex’], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{‘central’, ‘complex’, ‘multicomplex’, ‘forward’, ‘backward’}] defines the method used in the approximationorder : int, optional defines the order of the error term in the Taylor approximation used. For ‘central’ and ‘complex’ methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

hessdiag
[array] hessian diagonal

[47] https://docs.python.org/3.7/library/stdtypes.html#tuple

See also:

Derivative **(page 78),** *Hessian* **(page 85),** *Jacobian* **(page 88),** *Gradient* **(page 80)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

Lyness, J. M., Moler, C. B. (1966). Vandermonde Systems and Numerical
Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> fun = lambda x : x[0] + x[1]**2 + x[2]**3
>>> Hfun = nd.Hessdiag(fun, full_output=True)
>>> hd, info = Hfun([1,2,3])
>>> np.allclose(hd, [0.,   2.,  18.])
True
```

```
>>> np.all(info.error_estimate < 1e-11)
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

class info(*f_value*, *error_estimate*, *final_step*, *index*)

Bases: `tuple`[48]

count(*value*, */*)

Return number of occurrences of value.

property error_estimate

Alias for field number 1

property f_value

Alias for field number 0

property final_step

Alias for field number 2

property index

Alias for field number 3

property method

Defines the method used in the finite difference approximation.

property method_order

Defines the leading order of the error term in the Richardson extrapolation method.

property n

Order of the derivative.

property order

Defines the order of the error term in the Taylor approximation used.

set_richardson_rule(*step_ratio*, *num_terms=2*)

Set Richardson exptrapolation options

property step

The step spacing(s) used in the approximation

class Hessian(*f*, *step=None*, *method='central'*, *order=None*, ***options*)

Bases: *Hessdiag* (page 83)

Calculate Hessian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

[48] https://docs.python.org/3.7/library/stdtypes.html#tuple

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

hess
[ndarray] array of partial second derivatives, Hessian

See also:

Derivative **(page 78),** *Hessian* **(page 85)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Computes the Hessian according to method as: 'forward' (4.7), 'central' (4.9) and 'complex' (4.10):

$$((f(x + d_j e_j + d_k e_k) + f(x) - f(x + d_j e_j) - f(x + d_k e_k)))/(d_j d_k) \tag{5.4}$$

$$((f(x + d_j e_j + d_k e_k) - f(x + d_j e_j - d_k e_k)) - (f(x - d_j e_j + d_k e_k) - f(x - d_j e_j - d_k e_k))/(4 d_j d_k) \tag{5.5}$$

$$imag(f(x + i d_j e_j + d_k e_k) - f(x + i d_j e_j - d_k e_k))/(2 d_j d_k) \tag{5.6}$$

where e_j is a vector with element j is one and the rest are zero and d_j is a scalar spacing $steps_j$.

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

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Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nd.Hessian(rosen)
>>> h = Hfun([1, 1])
>>> h
array([[ 842., -420.],
       [-420.,  210.]])
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nd.Hessian(fun)
>>> h2 = Hfun2([0, 0])
>>> h2
array([[-1.,  1.],
       [ 1., -1.]])
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

class info(*f_value*, *error_estimate*, *final_step*, *index*)

Bases: `tuple`[49]

count(*value*, */*)

Return number of occurrences of value.

property error_estimate

Alias for field number 1

property f_value

Alias for field number 0

property final_step

Alias for field number 2

property index

Alias for field number 3

property method

Defines the method used in the finite difference approximation.

property method_order

Defines the leading order of the error term in the Richardson extrapolation method.

property n

Order of the derivative.

property order

Defines the order of the error term in the Taylor approximation used.

set_richardson_rule(*step_ratio*, *num_terms=2*)

Set Richardson exptrapolation options

property step

The step spacing(s) used in the approximation

class Jacobian(*fun*, *step=None*, *method='central'*, *order=2*, *n=1*, ***options*)

Bases: *Derivative* (page 78)

Calculate Jacobian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, array-like or StepGenerator object, optional] Defines the spacing used in the approximation. Default is MinStepGenerator(**step_options) if method in in ['complex', 'multicomplex'], otherwise

MaxStepGenerator(**step_options)

The results are extrapolated if the StepGenerator generate more than 3 steps.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

richardson_terms: scalar integer, default 2.
number of terms used in the Richardson extrapolation.

full_output
[bool, optional] If *full_output* is False, only the derivative is returned. If *full_output* is True, then (der, r) is returned *der* is the derivative, and *r* is a Results object.

****step_options:**
options to pass on to the XXXStepGenerator used.

Returns

jacob
[array] Jacobian

See also:

Derivative **(page 78),** *Hessian* **(page 85),** *Gradient* **(page 80)**

Notes

Complex methods are usually the most accurate provided the function to differentiate is analytic. The complex-step methods also requires fewer steps than the other methods and can work very close to the support of a function. The complex-step derivative has truncation error O(steps**2) for *n=1* and O(steps**4) for *n* larger, so truncation error can be eliminated by choosing steps to be very small. Especially the first order complex-step derivative avoids the problem of round-off error with small steps because there is no subtraction. However, this method fails if fun(x) does not support complex numbers or involves non-analytic functions such as e.g.: abs, max, min. Central difference methods are almost as accurate and has no restriction on type of function. For this reason the 'central' method is the default method, but sometimes one can only allow evaluation in forward or backward direction.

[49] https://docs.python.org/3.7/library/stdtypes.html#tuple

For all methods one should be careful in decreasing the step size too much due to round-off errors.

Higher order approximation methods will generally be more accurate, but may also suffer more from numerical problems. First order methods is usually not recommended.

If fun returns a 1d array, it returns a Jacobian. If a 2d array is returned by fun (e.g., with a value for each observation), it returns a 3d array with the Jacobian of each observation with shape xk x nobs x xk. I.e., the Jacobian of the first observation would be [:, 0, :]

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

K.-L. Lai, J.L. Crassidis, Y. Cheng, J. Kim (2005), New complex step
derivative approximations with application to second-order kalman filtering, AIAA Guidance, Navigation and Control Conference, San Francisco, California, August 2005, AIAA-2005-5944.

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Differentiation. *Numerische Mathematik*.

Lyness, J. M., Moler, C. B. (1969). Generalized Romberg Methods for
Integrals of Derivatives. *Numerische Mathematik*.

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape,  (10,))
True
```

```
>>> jfun = nd.Jacobian(fun)
>>> val = jfun([1, 2, 0.75])
>>> np.allclose(val, np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> jfun2 = nd.Jacobian(fun2)
>>> np.allclose(jfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
>>> jfun3 = nd.Jacobian(fun3)
```

```
>>> np.allclose(jfun3([1., 2., 3.]), [[[18.], [9.], [12.]], [[6.], [3.], [2.]]])
True
>>> np.allclose(jfun3([4., 5., 6.]), [[[180.], [144.], [240.]], [[30.], [24.],␣
↪[20.]]])
True
>>> np.allclose(jfun3(np.array([[1.,2.,3.]]).T), [[[18.], [9.], [12.]], [[6.],␣
↪[3.], [2.]]])
True
```

Methods

`__call__`(x, *args, **kwds)	Call self as a function.

class info(*f_value*, *error_estimate*, *final_step*, *index*)

Bases: `tuple`[50]

count(*value*, /)

Return number of occurrences of value.

property error_estimate

Alias for field number 1

property f_value

Alias for field number 0

property final_step

Alias for field number 2

property index

Alias for field number 3

property method

Defines the method used in the finite difference approximation.

property method_order

Defines the leading order of the error term in the Richardson extrapolation method.

property n

Order of the derivative.

property order

Defines the order of the error term in the Taylor approximation used.

set_richardson_rule(*step_ratio*, *num_terms=2*)

Set Richardson exptrapolation options

property step

The step spacing(s) used in the approximation

class MaxStepGenerator(*base_step=2.0*, *step_ratio=None*, *num_steps=15*, *step_nom=None*, *offset=0*, *num_extrap=9*, *use_exact_steps=False*, *check_num_steps=True*, *scale=500*)

Bases: *MinStepGenerator* (page 133)

Generates a sequence of steps

where

steps = step_nom * base_step * step_ratio ** (-i + offset)

for i = 0, 1, . . . , num_steps-1.

Parameters

base_step
: [float, array-like, default 2.0] Defines the maximum step, if None, the value is set to EPS**(1/scale)

step_ratio
: [real scalar, optional, default 2 or 1.6] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

[50] https://docs.python.org/3.7/library/stdtypes.html#tuple

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, default 500] scale used in base step.

`property base_step`
Base step defines the minimum or maximum step when offset==0.

`property min_num_steps`
Minimum number of steps required given the differentiation method and order.

`property num_steps`
Defines number of steps generated

`property scale`
Scale used in base step.

`step_generator_function`(*x*, *method='forward'*, *n=1*, *order=2*)
Step generator function

`property step_nom`
Nominal step

`property step_ratio`
Ratio between sequential steps generated

`class MinStepGenerator`(*base_step=None*, *step_ratio=None*, *num_steps=None*, *step_nom=None*, *offset=0*, *num_extrap=0*, *use_exact_steps=True*, *check_num_steps=True*, *scale=None*)

Bases: `object`[51]

Generates a sequence of steps

where
steps = step_nom * base_step * step_ratio ** (i + offset)

for i = num_steps-1,... 1, 0.

Parameters

base_step
[float, array-like, optional] Defines the minimum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 2] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, optional] scale used in base step. If not None it will override the default computed with the default_scale function.

`property base_step`

Base step defines the minimum or maximum step when offset==0.

`property min_num_steps`

Minimum number of steps required given the differentiation method and order.

`property num_steps`

Defines number of steps generated

`property scale`

Scale used in base step.

`step_generator_function`(*x*, *method='forward'*, *n=1*, *order=2*)

Step generator function

`property step_nom`

Nominal step

`property step_ratio`

Ratio between sequential steps generated

`class Richardson`(*step_ratio=2.0*, *step=1*, *order=1*, *num_terms=2*)

Bases: `object`[52]

Extrapolates a sequence with Richardsons method

Parameters

step_ratio: real scalar
Ratio between sequential steps, h, generated.

step: scalar integer
Defines the step between exponents in the error polynomial, i.e., step = k_1 - k_0 = k_2 - k_1 = … = k_{i+1} - k_i

order: scalar integer
Leading order of truncation error.

[51] https://docs.python.org/3.7/library/functions.html#object

num_terms: scalar integer
Number of terms used in the polynomial fit.

Notes

Suppose f(h) is an approximation of L (exact value) that depends on a positive step size h described with a sequence of the form

L = f(h) + a0 * h^k_0 + a1 * h^k_1+ a2 * h^k_2 + ...

where the ai are unknown constants and the k_i are known constants such that h^k_i > h^(k_i+1).

If we evaluate the right hand side for different stepsizes h we can fit a polynomial to that sequence of approximations. This is exactly what this class does. Here k_0 is the leading order step size behavior of truncation error as L = f(h)+O(h^k_0) (f(h) -> L as h -> 0, but f(0) != L) and k_i = order + step * i .

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> n = 3
>>> Ei = np.zeros((n,1))
>>> h = np.zeros((n,1))
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(n):
...     x = linfun(k)
...     h[k] = x[1]
...     Ei[k] = np.trapz(np.sin(x),x)
>>> En, err, step = nd.Richardson(step=1, order=1)(Ei, h)
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
>>> np.allclose(En, 1)
True
```

extrapolate(*sequence*, *steps*)
Extrapolate sequence

rule(*sequence_length=None*)
Returns extrapolation rule.

dea3(*v_0*, *v_1*, *v_2*, *symmetric=False*)
Extrapolate a slowly convergent sequence using Shanks transformations.

Parameters

v_0, v_1, v_2
[array-like] 3 values of a convergent sequence to extrapolate

Returns

result
[array-like] extrapolated value

abserr
[array-like] absolute error estimate

See also:

[52] https://docs.python.org/3.7/library/functions.html#object

Dea

Notes

DEA3 attempts to extrapolate nonlinearly by Shanks transformations to a better estimate of the sequence's limiting value based on only three values. The epsilon algorithm of P. Wynn, see [Rf7ab399ffe8b-1], is used to perform the non-linear Shanks transformations. The routine is a vectorized translation of the DQELG function found in the QUADPACK fortran library for LIMEXP=3, see [Rf7ab399ffe8b-2] and [Rf7ab399ffe8b-3].

References

Examples

integrate sin(x) from 0 to pi/2

```
>>> import numpy as np
>>> import numdifftools as nd
>>> Ei= np.zeros(3)
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(3):
...     x = linfun(k)
...     Ei[k] = np.trapz(np.sin(x),x)
>>> [En, err] = nd.dea3(Ei[0], Ei[1], Ei[2])
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.allclose(En, 1)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
```

directionaldiff(*f*, *x0*, *vec*, ***options*)

Return directional derivative of a function of n variables

Parameters

f: function
analytical function to differentiate.

x0: array
vector location at which to differentiate 'f'. If x0 is an nXm array, then 'f' is assumed to be a function of n*m variables.

vec: array
vector defining the line along which to take the derivative. It should be the same size as x0, but need not be a vector of unit length.

****options:**
optional arguments to pass on to Derivative.

Returns

dder: scalar
estimate of the first derivative of 'f' in the specified direction.

See also:

Derivative **(page 78)**
Gradient **(page 80)**

Examples

At the global minimizer (1,1) of the Rosenbrock function, compute the directional derivative in the direction [1 2]

```
>>> import numpy as np
>>> import numdifftools as nd
>>> vec = np.r_[1, 2]
>>> rosen = lambda x: (1-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> dd, info = nd.directionaldiff(rosen, [1, 1], vec, full_output=True)
>>> np.allclose(dd, 0)
True
>>> np.abs(info.error_estimate)<1e-14
True
```

5.2.3 numdifftools.extrapolation module

Created on 28. aug. 2015

@author: pab

class Dea(*limexp=50*)

Bases: object[53]

Extrapolate a slowly convergent sequence using repeated Shanks transformations.

Notes

DEA attempts to extrapolate nonlinearly by Shanks transformations to a better estimate of the sequence's limiting value, thus improving the rate of convergence. The epsilon algorithm of P. Wynn, see [1]_, is used to perform the non-linear Shanks transformations. The routine is a translation of the DQELG function found in the QUADPACK fortran library, see [2]_ and [3]_.

List of major variables:

LIMEXP: scalar integer
The maximum number of elements the epsilon table data can contain. The epsilon table is stored in the first (LIMEXP+2) entries of EPSTAB.

EPSTAB: real vector or size (LIMEXP+2+3)

The first LIMEXP+2 elements contains the two lower diagonals of the triangular epsilon table. The elements are numbered starting at the right-hand corner of the

triangle.

E0,E1,E2,E3: real scalars
The 4 elements on which the computation of a new element in the epsilon table is based.

NRES: scalar integer
Number of extrapolation results actually generated by the epsilon algorithm in prior calls to the routine.

NEWELM: scalar integer
Number of elements to be computed in the new diagonal of the epsilon table. The condensed epsilon table is computed. Only those elements needed for the computation of the next diagonal are preserved.

RES: real scalar
New element in the new diagonal of the epsilon table.

ERROR: real scalar
An estimate of the absolute error of RES. The routine decides whether RESULT=RES or RESULT=SVALUE by comparing ERROR with abserr from the previous call.

RES3LA: real vector of size 3
Contains at most the last 3 results.

`property limexp`

Maximum number of elements the epsilon table data.

`class EpsAlg`

Bases: `object`[54]

Extrapolate a slowly convergent sequence using Shanks transformation.

Notes

The iterated Shanks transformation is computed using the Wynn epsilon algorithm (see equation 4.3-10a to 4.3-10c given on page 25 in [R9678172c97e0-1]).

References

`class Richardson`(*step_ratio=2.0*, *step=1*, *order=1*, *num_terms=2*)

Bases: `object`[55]

Extrapolates a sequence with Richardsons method

Parameters

step_ratio: real scalar
Ratio between sequential steps, h, generated.

step: scalar integer
Defines the step between exponents in the error polynomial, i.e., step = k_1 - k_0 = k_2 - k_1 = … = k_{i+1} - k_i

order: scalar integer
Leading order of truncation error.

num_terms: scalar integer
Number of terms used in the polynomial fit.

Notes

Suppose f(h) is an approximation of L (exact value) that depends on a positive step size h described with a sequence of the form

L = f(h) + a0 * h^k_0 + a1 * h^k_1+ a2 * h^k_2 + …

where the ai are unknown constants and the k_i are known constants such that h^k_i > h^(k_i+1).

If we evaluate the right hand side for different stepsizes h we can fit a polynomial to that sequence of approximations. This is exactly what this class does. Here k_0 is the leading order step size behavior of truncation error as L = f(h)+O(h^k_0) (f(h) -> L as h -> 0, but f(0) != L) and k_i = order + step * i .

[53] https://docs.python.org/3.7/library/functions.html#object
[54] https://docs.python.org/3.7/library/functions.html#object

Examples

```
>>> import numpy as np
>>> import numdifftools as nd
>>> n = 3
>>> Ei = np.zeros((n,1))
>>> h = np.zeros((n,1))
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(n):
...     x = linfun(k)
...     h[k] = x[1]
...     Ei[k] = np.trapz(np.sin(x),x)
>>> En, err, step = nd.Richardson(step=1, order=1)(Ei, h)
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
>>> np.allclose(En, 1)
True
```

extrapolate(*sequence*, *steps*)

Extrapolate sequence

rule(*sequence_length=None*)

Returns extrapolation rule.

convolve(*sequence*, *rule*, ***kwds*)

Wrapper around scipy.ndimage.convolve1d that allows complex input.

dea3(*v_0*, *v_1*, *v_2*, *symmetric=False*)

Extrapolate a slowly convergent sequence using Shanks transformations.

Parameters

v_0, v_1, v_2
[array-like] 3 values of a convergent sequence to extrapolate

Returns

result
[array-like] extrapolated value

abserr
[array-like] absolute error estimate

See also:

Dea **(page 95)**

[55] https://docs.python.org/3.7/library/functions.html#object

Notes

DEA3 attempts to extrapolate nonlinearly by Shanks transformations to a better estimate of the sequence's limiting value based on only three values. The epsilon algorithm of P. Wynn, see [Rc8bfc08f7c28-1], is used to perform the non-linear Shanks transformations. The routine is a vectorized translation of the DQELG function found in the QUADPACK fortran library for LIMEXP=3, see [Rc8bfc08f7c28-2] and [Rc8bfc08f7c28-3].

References

Examples

integrate sin(x) from 0 to pi/2

```
>>> import numpy as np
>>> import numdifftools as nd
>>> Ei= np.zeros(3)
>>> linfun = lambda i : np.linspace(0, np.pi/2., 2**(i+5)+1)
>>> for k in np.arange(3):
...     x = linfun(k)
...     Ei[k] = np.trapz(np.sin(x),x)
>>> [En, err] = nd.dea3(Ei[0], Ei[1], Ei[2])
>>> truErr = np.abs(En-1.)
>>> np.all(truErr < err)
True
>>> np.allclose(En, 1)
True
>>> np.all(np.abs(Ei-1)<1e-3)
True
```

dea_demo()

```
>>> from numdifftools.extrapolation import dea_demo
>>> dea_demo()
NO. PANELS      TRAP. APPROX          APPROX W/EA           abserr
    1           0.78539816            0.78539816            0.78539816
    2           0.94805945            0.94805945            0.97596771
    4           0.98711580            0.99945672            0.21405856
    8           0.99678517            0.99996674            0.05190729
   16           0.99919668            0.99999988            0.00057629
   32           0.99979919            1.00000000            0.00057665
   64           0.99994980            1.00000000            0.00003338
  128           0.99998745            1.00000000            0.00000012
  256           0.99999686            1.00000000            0.00000000
  512           0.99999922            1.00000000            0.00000000
 1024           0.99999980            1.00000000            0.00000000
 2048           0.99999995            1.00000000            0.00000000
```

epsalg_demo()

```
>>> from numdifftools.extrapolation import epsalg_demo
>>> epsalg_demo()
NO. PANELS      TRAP. APPROX          APPROX W/EA           abserr
    1           0.78539816            0.78539816            0.21460184
    2           0.94805945            0.94805945            0.05194055
    4           0.98711580            0.99945672            0.00054328
    8           0.99678517            0.99996674            0.00003326
```

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```
  16          0.99919668          0.99999988          0.00000012
  32          0.99979919          1.00000000          0.00000000
  64          0.99994980          1.00000000          0.00000000
 128          0.99998745          1.00000000          0.00000000
 256          0.99999686          1.00000000          0.00000000
 512          0.99999922          1.00000000          0.00000000
```

max_abs(*a*, *b*)

Returns element-wise maximum of absulute value of array elements

richardson_demo()

```
>>> from numdifftools.extrapolation import richardson_demo
>>> richardson_demo()
NO. PANELS      TRAP. APPROX          APPROX W/R            abserr
    1           0.78539816          0.78539816          0.21460184
    2           0.94805945          1.11072073          0.11072073
    4           0.98711580          0.99798929          0.00201071
    8           0.99678517          0.99988201          0.00011799
   16           0.99919668          0.99999274          0.00000726
   32           0.99979919          0.99999955          0.00000045
   64           0.99994980          0.99999997          0.00000003
  128           0.99998745          1.00000000          0.00000000
  256           0.99999686          1.00000000          0.00000000
  512           0.99999922          1.00000000          0.00000000
```

5.2.4 numdifftools.finite_difference module

Finite difference methods module.

class DifferenceFunctions

Bases: object[56]

Class defining difference functions

Notes

The d

class HessdiagDifferenceFunctions

Bases: object[57]

Class defining Hessdiag difference functions

References

Ridout, M.S. (2009) Statistical applications of the complex-step method
of numerical differentiation. The American Statistician, 63, 66-74

class HessianDifferenceFunctions

Bases: object[58]

Class defining Hessian difference functions

[56] https://docs.python.org/3.7/library/functions.html#object
[57] https://docs.python.org/3.7/library/functions.html#object

References

Ridout, M.S. (2009) "Statistical applications of the complex-step method of numerical differentiation", The American Statistician, 63, 66-74

class JacobianDifferenceFunctions

Bases: object[59]

Class defining Jacobian difference functions

static increments(*n*, *h*)

Returns Jacobian steps

class LogHessdiagRule(*n=1*, *method='central'*, *order=2*)

Bases: *LogRule* (page 102)

Log spaced finite difference Hessdiag rule class

Parameters

n
[2] Order of the derivative.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

Examples

```
>>> import numpy as np
>>> from numdifftools.finite_difference import LogHessdiagRule as Rule
```

```
>>> np.allclose(Rule(method='central', order=2).rule(step_ratio=2.0), 2)
True
>>> np.allclose(Rule(method='central', order=4).rule(step_ratio=2.),
...             [-0.66666667, 10.66666667])
True
>>> np.allclose(Rule(method='central', order=6).rule(step_ratio=2.),
...             [ 4.44444444e-02, -3.55555556e+00,  4.55111111e+01])
True
>>> np.allclose(Rule(method='forward', order=2).rule(step_ratio=2.), [ -4.,  40.,
↪ -64.])
True
>>> np.allclose(Rule(method='forward', order=4).rule(step_ratio=2.),
...          [-1.90476190e-01,  1.10476190e+01, -1.92000000e+02,
...          1.12152381e+03, -1.56038095e+03])
True
>>> np.allclose(Rule(method='forward', order=6).rule(step_ratio=2.),
...    [-4.09626216e-04,  1.02406554e-01, -8.33015873e+00,  2.76317460e+02,
...     -3.84893968e+03,  2.04024004e+04, -2.74895500e+04])
True
>>> step_ratio=2.0
>>> fd_rule = Rule(method='forward', order=4)
```

(continues on next page)

[58] https://docs.python.org/3.7/library/functions.html#object
[59] https://docs.python.org/3.7/library/functions.html#object

(continued from previous page)

```
>>> steps = 0.002*(1./step_ratio)**np.arange(6)
>>> x0 = np.array([0., 0.])
>>> f = lambda xy : np.cos(xy[0]-xy[1])
>>> f_x0 = f(x0)
>>> f_del = [f(x0+h) - f_x0  for h in steps] # forward difference
>>> f_del = [fd_rule.diff(f, f_x0, x0, h) for h in steps]  # or alternatively
>>> fder, h, shape = fd_rule.apply(f_del, steps, step_ratio)
```

```
>>> np.allclose(fder, [[-1., -1.], [-1., -1.]])
True
```

property n

class LogHessianRule(*n=1*, *method='central'*, *order=2*)

Bases: *LogRule* (page 102)

Log spaced finite difference Hessian rule class

Parameters

n
[2] Order of the derivative.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

apply(*sequence*, *steps*, *step_ratio=2.0*)

Apply finite difference rule along the first axis.

Return derivative estimates of fun at x0 for a sequence of stepsizes h

Parameters

sequence: finite differences
steps: steps

property n

property order

The order of the error term in the Taylor approximation used

class LogJacobianRule(*n=1*, *method='central'*, *order=2*)

Bases: *LogRule* (page 102)

Log spaced finite difference Jacobian rule class

Parameters

n
[1] Order of the derivative.

method
[{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
[int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

Examples

```
>>> from numdifftools.finite_difference import LogJacobianRule as Rule
>>> np.allclose(Rule(n=1, method='central', order=2).rule(step_ratio=2.0), 1)
True
>>> np.allclose(Rule(n=1, method='central', order=4).rule(step_ratio=2.),
...             [-0.33333333,  2.66666667])
True
>>> np.allclose(Rule(n=1, method='central', order=6).rule(step_ratio=2.),
...             [ 0.02222222, -0.88888889,  5.68888889])
True
```

```
>>> np.allclose(Rule(n=1, method='forward', order=2).rule(step_ratio=2.), [-1., ␣
↪4.])
True
```

```
>>> np.allclose(Rule(n=1, method='forward', order=4).rule(step_ratio=2.),
...             [ -0.04761905,   1.33333333, -10.66666667,  24.38095238])
True
>>> np.allclose(Rule(n=1, method='forward', order=6).rule(step_ratio=2.),
...    [ -1.02406554e-04,   1.26984127e-02,  -5.07936508e-01,
...       8.12698413e+00,  -5.20126984e+01,   1.07381055e+02])
True
>>> step_ratio=2.0
>>> fd_rule = Rule(n=1, method='forward', order=4)
>>> steps = 0.002*(1./step_ratio)**np.arange(6)
```

```
>>> x0 = np.atleast_1d(1.)
>>> f = np.exp
>>> f_x0 = f(x0)
>>> f_del = [f(x0+h) - f_x0  for h in steps] # forward difference
>>> f_del = [fd_rule.diff(f, f_x0, x0, h) for h in steps[:, None]]  # or␣
↪alternatively
>>> fder, h, shape = fd_rule.apply(f_del, steps, step_ratio)
>>> np.allclose(fder, f(x0))
True
```

class LogRule(*n=1*, *method='central'*, *order=2*)

Bases: object[60]

Log spaced finite difference rule class

Parameters

n
: [int, optional] Order of the derivative.

method
: [{'central', 'complex', 'multicomplex', 'forward', 'backward'}] defines the method used in the approximation

order
: [int, optional] defines the order of the error term in the Taylor approximation used. For 'central' and 'complex' methods, it must be an even number.

Examples

```
>>> from numdifftools.finite_difference import LogRule
>>> np.allclose(LogRule(n=1, method='central', order=2).rule(step_ratio=2.0), 1)
True
>>> np.allclose(LogRule(n=1, method='central', order=4).rule(step_ratio=2.),
...             [-0.33333333,  2.66666667])
True
>>> np.allclose(LogRule(n=1, method='central', order=6).rule(step_ratio=2.),
...             [ 0.02222222, -0.88888889,  5.68888889])
True
```

```
>>> np.allclose(LogRule(n=1, method='forward', order=2).rule(step_ratio=2.), [-1.
↪,  4.])
True
```

```
>>> np.allclose(LogRule(n=1, method='forward', order=4).rule(step_ratio=2.),
...             [ -0.04761905,   1.33333333, -10.66666667,  24.38095238])
True
>>> np.allclose(LogRule(n=1, method='forward', order=6).rule(step_ratio=2.),
...    [ -1.02406554e-04,   1.26984127e-02,  -5.07936508e-01,
...       8.12698413e+00,  -5.20126984e+01,   1.07381055e+02])
True
>>> step_ratio=2.0
>>> fd_rule = LogRule(n=2, method='forward', order=4)
>>> h = 0.002*(1./step_ratio)**np.arange(6)
>>> x0 = 1.
>>> f = np.exp
>>> f_x0 = f(x0)
>>> f_del = f(x0+h) - f_x0  # forward difference
>>> f_del = fd_rule.diff(f, f_x0, x0, h)  # or alternatively
>>> fder, h, shape = fd_rule.apply(f_del, h, step_ratio)
>>> np.allclose(fder, f(x0))
True
```

apply(*sequence*, *steps*, *step_ratio=2.0*)

Apply finite difference rule along the first axis.

Return derivative estimates of fun at x0 for a sequence of stepsizes h

Parameters

sequence: finite differences
steps: steps

property diff

The difference function

property eval_first_condition

True if f(x0) needs to be evaluated given the differentiation method.

property method_order

The leading order of the truncation error of the Richardson extrapolation.

property richardson_step

The step between exponents in the error polynomial of the Richardson extrapolation.

rule(*step_ratio=2.0*)

Return finite differencing rule.

Parameters

step_ratio
[real scalar, optional, default 2.0] Ratio between sequential steps generated.

Notes

The rule is for a nominal unit step size, and must be scaled later to reflect the local step size.

Member method used: _fd_matrix

Member variables used: n order method

`make_exact`(*h*)

Make sure h is an exact representable number

This is important when calculating numerical derivatives and is accomplished by adding 1.0 and then subtracting 1.0.

5.2.5 numdifftools.fornberg module

`class Taylor`(*fun*, *n=1*, *r=0.0059*, *num_extrap=3*, *step_ratio=1.6*, ***kwds*)

Bases: `object`[61]

Return Taylor coefficients of complex analytic function using FFT

Parameters

fun
[callable] function to differentiate

z0
[real or complex scalar at which to evaluate the derivatives]

n
[scalar integer, default 1] Number of taylor coefficents to compute. Maximum number is 100.

r
[real scalar, default 0.0059] Initial radius at which to evaluate. For well-behaved functions, the computation should be insensitive to the initial radius to within about four orders of magnitude.

num_extrap
[scalar integer, default 3] number of extrapolation steps used in the calculation

step_ratio
[real scalar, default 1.6] Initial grow/shrinking factor for finding the best radius.

max_iter
[scalar integer, default 30] Maximum number of iterations

min_iter
[scalar integer, default max_iter // 2] Minimum number of iterations before the solution may be deemed degenerate. A larger number allows the algorithm to correct a bad initial radius.

full_output
[bool, optional] If *full_output* is False, only the coefficents is returned (default). If *full_output* is True, then (coefs, status) is returned

Returns

[60] https://docs.python.org/3.7/library/functions.html#object

coefs
[ndarray] array of taylor coefficents

status: Optional object into which output information is written:
degenerate: True if the algorithm was unable to bound the error iterations: Number of iterations executed function_count: Number of function calls final_radius: Ending radius of the algorithm failed: True if the maximum number of iterations was reached error_estimate: approximate bounds of the rounding error.

Notes

This module uses the method of Fornberg to compute the Taylor series coefficients of a complex analytic function along with error bounds. The method uses a Fast Fourier Transform to invert function evaluations around a circle into Taylor series coefficients and uses Richardson Extrapolation to improve and bound the estimate. Unlike real-valued finite differences, the method searches for a desirable radius and so is reasonably insensitive to the initial radius-to within a number of orders of magnitude at least. For most cases, the default configuration is likely to succeed.

Restrictions: The method uses the coefficients themselves to control the truncation error, so the error will not be properly bounded for functions like low-order polynomials whose Taylor series coefficients are nearly zero. If the error cannot be bounded, degenerate flag will be set to true, and an answer will still be computed and returned but should be used with caution.

References

[1] Fornberg, B. (1981).
Numerical Differentiation of Analytic Functions. ACM Transactions on Mathematical Software (TOMS), 7(4), 512-526. http://doi.org/10.1145/355972.355979

Examples

Compute the first 6 taylor coefficients 1 / (1 - z) expanded round z0 = 0:

```
>>> import numdifftools.fornberg as ndf
>>> import numpy as np
>>> c, info = ndf.Taylor(lambda x: 1./(1-x), n=6, full_output=True)(z0=0)
>>> np.allclose(c, np.ones(8))
True
>>> np.all(info.error_estimate < 1e-9)
True
>>> (info.function_count, info.iterations, info.failed) == (136, 17, False)
True
```

derivative(*fun*, *z0*, *n=1*, ***kwds*)

Calculate n-th derivative of complex analytic function using FFT

Parameters

fun
[callable] function to differentiate

z0
[real or complex scalar at which to evaluate the derivatives]

n
[scalar integer, default 1] Number of derivatives to compute where 0 represents the value of the function and n represents the nth derivative. Maximum number is 100.

[61] https://docs.python.org/3.7/library/functions.html#object

r
: [real scalar, default 0.0061] Initial radius at which to evaluate. For well-behaved functions, the computation should be insensitive to the initial radius to within about four orders of magnitude.

max_iter
: [scalar integer, default 30] Maximum number of iterations

min_iter
: [scalar integer, default max_iter // 2] Minimum number of iterations before the solution may be deemed degenerate. A larger number allows the algorithm to correct a bad initial radius.

step_ratio
: [real scalar, default 1.6] Initial grow/shrinking factor for finding the best radius.

num_extrap
: [scalar integer, default 3] number of extrapolation steps used in the calculation

full_output
: [bool, optional] If *full_output* is False, only the derivative is returned (default). If *full_output* is True, then (der, status) is returned *der* is the derivative, and *status* is a Results object.

Returns

der
: [ndarray] array of derivatives

status: Optional object into which output information is written. Fields:
: degenerate: True if the algorithm was unable to bound the error iterations: Number of iterations executed function_count: Number of function calls final_radius: Ending radius of the algorithm failed: True if the maximum number of iterations was reached error_estimate: approximate bounds of the rounding error.

Notes

This module uses the method of Fornberg to compute the derivatives of a complex analytic function along with error bounds. The method uses a Fast Fourier Transform to invert function evaluations around a circle into Taylor series coefficients, uses Richardson Extrapolation to improve and bound the estimate, then multiplies by a factorial to compute the derivatives. Unlike real-valued finite differences, the method searches for a desirable radius and so is reasonably insensitive to the initial radius-to within a number of orders of magnitude at least. For most cases, the default configuration is likely to succeed.

Restrictions: The method uses the coefficients themselves to control the truncation error, so the error will not be properly bounded for functions like low-order polynomials whose Taylor series coefficients are nearly zero. If the error cannot be bounded, degenerate flag will be set to true, and an answer will still be computed and returned but should be used with caution.

References

[1] Fornberg, B. (1981).
Numerical Differentiation of Analytic Functions. ACM Transactions on Mathematical Software (TOMS), 7(4), 512-526. http://doi.org/10.1145/355972.355979

Examples

To compute the first five derivatives of 1 / (1 - z) at z = 0: Compute the first 6 taylor derivatives of 1 / (1 - z) at z0 = 0:

```
>>> import numdifftools.fornberg as ndf
>>> import numpy as np
>>> def fun(x):
...     return 1./(1-x)
>>> c, info = ndf.derivative(fun, z0=0, n=6, full_output=True)
>>> np.allclose(c, [1, 1, 2, 6, 24, 120, 720, 5040])
True
>>> np.all(info.error_estimate < 1e-9*c.real)
True
>>> (info.function_count, info.iterations, info.failed) == (136, 17, False)
True
```

fd_derivative(*fx*, *x*, *n=1*, *m=2*)

Return the n'th derivative for all points using Finite Difference method.

Parameters

fx
: [vector] function values which are evaluated on x i.e. fx[i] = f(x[i])

x
: [vector] abscissas on which fx is evaluated. The x values can be arbitrarily spaced but must be distinct and len(x) > n.

n
: [scalar integer] order of derivative.

m
: [scalar integer] defines the stencil size. The stencil size is of 2 * mm + 1 points in the interior, and 2 * mm + 2 points for each of the 2 * mm boundary points where mm = n // 2 + m.

fd_derivative evaluates an approximation for the n'th derivative of the vector function f(x) using the Fornberg finite difference method. Restrictions: 0 < n < len(x) and 2*mm+2 <= len(x)

See also:

fd_weights **(page 107)**

Examples

```
>>> import numpy as np
>>> import numdifftools.fornberg as ndf
>>> x = np.linspace(-1, 1, 25)
>>> fx = np.exp(x)
>>> df = ndf.fd_derivative(fx, x, n=1)
>>> np.allclose(df, fx)
True
```

fd_weights(*x*, *x0=0*, *n=1*)

Return finite difference weights for the n'th derivative.

Parameters

x
: [vector] abscissas used for the evaluation for the derivative at x0.

x0
: [scalar] location where approximations are to be accurate

n
: [scalar integer] order of derivative. Note for n=0 this can be used to evaluate the interpolating polynomial itself.

See also:

fd_weights_all **(page 108)**

Examples

```
>>> import numpy as np
>>> import numdifftools.fornberg as ndf
>>> x = np.linspace(-1, 1, 5) * 1e-3
>>> w = ndf.fd_weights(x, x0=0, n=1)
>>> df = np.dot(w, np.exp(x))
>>> np.allclose(df, 1)
True
```

fd_weights_all(*x*, *x0=0*, *n=1*)

Return finite difference weights for derivatives of all orders up to n.

Parameters

x
: [vector, length m] x-coordinates for grid points

x0
: [scalar] location where approximations are to be accurate

n
: [scalar integer] highest derivative that we want to find weights for

Returns

weights
: [array, shape n+1 x m] contains coefficients for the j'th derivative in row j (0 <= j <= n)

See also:

fd_weights **(page 107)**

Notes

The x values can be arbitrarily spaced but must be distinct and len(x) > n.

The Fornberg algorithm is much more stable numerically than regular vandermonde systems for large values of n.

References

B. Fornberg (1998) "Calculation of weights_and_points in finite difference formulas", SIAM Review 40, pp. 685-691.

http://www.scholarpedia.org/article/Finite_difference_method

`richardson`(*vals*, *k*, *c=None*)

Richardson extrapolation with parameter estimation

`richardson_parameter`(*vals*, *k*)

`taylor`(*fun*, *z0=0*, *n=1*, *r=0.0059*, *num_extrap=3*, *step_ratio=1.6*, ***kwds*)

Return Taylor coefficients of complex analytic function using FFT

Parameters

fun
[callable] function to differentiate

z0
[real or complex scalar at which to evaluate the derivatives]

n
[scalar integer, default 1] Number of taylor coefficents to compute. Maximum number is 100.

r
[real scalar, default 0.0059] Initial radius at which to evaluate. For well-behaved functions, the computation should be insensitive to the initial radius to within about four orders of magnitude.

num_extrap
[scalar integer, default 3] number of extrapolation steps used in the calculation

step_ratio
[real scalar, default 1.6] Initial grow/shrinking factor for finding the best radius.

max_iter
[scalar integer, default 30] Maximum number of iterations

min_iter
[scalar integer, default max_iter // 2] Minimum number of iterations before the solution may be deemed degenerate. A larger number allows the algorithm to correct a bad initial radius.

full_output
[bool, optional] If *full_output* is False, only the coefficents is returned (default). If *full_output* is True, then (coefs, status) is returned

Returns

coefs
[ndarray] array of taylor coefficents

status: Optional object into which output information is written:
degenerate: True if the algorithm was unable to bound the error iterations: Number of iterations executed function_count: Number of function calls final_radius: Ending radius of the algorithm failed: True if the maximum number of iterations was reached error_estimate: approximate bounds of the rounding error.

Notes

This module uses the method of Fornberg to compute the Taylor series coefficents of a complex analytic function along with error bounds. The method uses a Fast Fourier Transform to invert function evaluations around a circle into Taylor series coefficients and uses Richardson Extrapolation to improve and bound the estimate. Unlike real-valued finite differences, the method searches for a desirable radius and so is reasonably insensitive to the initial radius-to within a number of orders of magnitude at least. For most cases, the default configuration is likely to succeed.

Restrictions: The method uses the coefficients themselves to control the truncation error, so the error will not be properly bounded for functions like low-order polynomials whose Taylor series coefficients are nearly zero. If the error cannot be bounded, degenerate flag will be set to true, and an answer will still be computed and returned but should be used with caution.

References

[1] Fornberg, B. (1981).
Numerical Differentiation of Analytic Functions. ACM Transactions on Mathematical Software (TOMS), 7(4), 512-526. http://doi.org/10.1145/355972.355979

Examples

Compute the first 6 taylor coefficients 1 / (1 - z) expanded round z0 = 0:

```
>>> import numdifftools.fornberg as ndf
>>> import numpy as np
>>> c, info = ndf.taylor(lambda x: 1./(1-x), z0=0, n=6, full_output=True)
>>> np.allclose(c, np.ones(8))
True
>>> np.all(info.error_estimate < 1e-9)
True
>>> (info.function_count, info.iterations, info.failed) == (136, 17, False)
True
```

5.2.6 numdifftools.limits module

Created on 27. aug. 2015

@author: pab Author: John D'Errico e-mail: woodchips@rochester.rr.com Release: 1.0 Release date: 5/23/2008

class CStepGenerator(*base_step=None*, *step_ratio=4.0*, *num_steps=None*, *step_nom=None*, *offset=0*, *scale=1.2*, ***options*)

Bases: *MinStepGenerator* (page 133)

Generates a sequence of steps

where
steps = base_step * step_nom * (exp(1j*dtheta) * step_ratio) ** (i + offset)

for i = 0, 1, ..., num_steps-1

Parameters

base_step
[float, array-like, default None] Defines the minimum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 4.0] Ratio between sequential steps generated.

num_steps
[scalar integer, optional,] defines number of steps generated. If None the value is 2 * int(round(16.0/log(abs(step_ratio)))) + 1

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

use_exact_steps
[boolean, default True.] If true make sure exact steps are generated.

scale
[real scalar, default 1.2] scale used in base step.

path
[‘radial’ or ‘spiral’] Specifies the type of path to take the limit along. Default ‘radial’.

dtheta: real scalar, default pi/8
If the path is ‘spiral’ it will follow an exponential spiral into the limit, with angular steps at dtheta radians.

`property dtheta`

Angular steps in radians used for the exponential spiral path.

`property num_steps`

The number of steps generated

`property step_ratio`

Ratio between sequential steps generated.

`class Limit`(*fun*, *step=None*, *method='above'*, *order=4*, *full_output=False*, ***options*)

Bases: `_Limit`

Compute limit of a function at a given point

Parameters

fun
[callable] function fun(z, **args*, ***kwds*) to compute the limit for z->z0. The function, fun, is assumed to return a result of the same shape and size as its input, *z*.

step: float, complex, array-like or StepGenerator object, optional
Defines the spacing used in the approximation. Default is CStepGenerator(base_step=step, **options)

method
[{‘above’, ‘below’}] defines if the limit is taken from *above* or *below*

order: positive scalar integer, optional.
defines the order of approximation used to find the specified limit. The order must be member of [1 2 3 4 5 6 7 8]. 4 is a good compromise.

full_output: bool
If true return additional info.

options:
options to pass on to CStepGenerator

Returns

limit_fz: array like
estimated limit of f(z) as z –> z0

info:
Only given if full_output is True and contains the following:

error estimate: ndarray
95 % uncertainty estimate around the limit, such that abs(limit_fz - lim z->z0 f(z)) < error_estimate

final_step: ndarray
final step used in approximation

Notes

Limit computes the limit of a given function at a specified point, z0. When the function is evaluable at the point in question, this is a simple task. But when the function cannot be evaluated at that location due to a singularity, you may need a tool to compute the limit. *Limit* does this, as well as produce an uncertainty estimate in the final result.

The methods used by *Limit* are Richardson extrapolation in a combination with Wynn's epsilon algorithm which also yield an error estimate. The user can specify the method order, as well as the path into z0. z0 may be real or complex. *Limit* uses a proportionally cascaded series of function evaluations, moving away from your point of evaluation along a path along the real line (or in the complex plane for complex z0 or step.) The *step_ratio* is the ratio used between sequential steps. The sign of step allows you to specify a limit from above or below. Negative values of step will cause the limit to be taken approaching z0 from below.

A smaller *step_ratio* means that *Limit* will take more function evaluations to evaluate the limit, but the result will potentially be less accurate. The *step_ratio* MUST be a scalar larger than 1. A value in the range [2,100] is recommended. 4 seems a good compromise.

```
>>> import numpy as np
>>> from numdifftools.limits import Limit
>>> def f(x): return np.sin(x)/x
>>> lim_f0, err = Limit(f, full_output=True)(0)
>>> np.allclose(lim_f0, 1)
True
>>> np.allclose(err.error_estimate, 1.772494446109966e-15)
True
```

Compute the derivative of cos(x) at x == pi/2. It should be -1. The limit will be taken as a function of the differential parameter, dx.

```
>>> x0 = np.pi/2;
>>> def g(x): return (np.cos(x0+x)-np.cos(x0))/x
>>> lim_g0, err = Limit(g, full_output=True)(0)
>>> np.allclose(lim_g0, -1)
True
>>> err.error_estimate < 1e-14
True
```

Compute the residue at a first order pole at z = 0 The function 1./(1-exp(2*z)) has a pole at z == 0. The residue is given by the limit of z*fun(z) as z –> 0. Here, that residue should be -0.5.

```
>>> def h(z): return -z/(np.expm1(2*z))
>>> lim_h0, err = Limit(h, full_output=True)(0)
>>> np.allclose(lim_h0, -0.5)
True
>>> err.error_estimate < 1e-14
True
```

Compute the residue of function 1./sin(z)**2 at z = 0. This pole is of second order thus the residue is given by the limit of z**2*fun(z) as z –> 0.

```
>>> def g(z): return z**2/(np.sin(z)**2)
>>> lim_gpi, err = Limit(g, full_output=True)(0)
>>> np.allclose(lim_gpi, 1)
True
>>> err.error_estimate < 1e-14
True
```

A more difficult limit is one where there is significant subtractive cancellation at the limit point. In the following example, the cancellation is second order. The true limit should be 0.5.

```
>>> def k(x): return (x*np.exp(x)-np.expm1(x))/x**2
>>> lim_k0,err = Limit(k, full_output=True)(0)
>>> np.allclose(lim_k0, 0.5)
True
>>> err.error_estimate < 1.0e-8
True
```

```
>>> def h(x): return  (x-np.sin(x))/x**3
>>> lim_h0, err = Limit(h, full_output=True)(0)
>>> np.allclose(lim_h0, 1./6)
True
>>> err.error_estimate < 1e-8
True
```

limit(*x*, **args*, ***kwds*)

Return lim f(z) as z-> x

class Residue(*f*, *step=None*, *method='above'*, *order=None*, *pole_order=1*, *full_output=False*, ***options*)

Bases: *Limit* (page 111)

Compute residue of a function at a given point

Parameters

fun
[callable] function fun(z, **args*, ***kwds*) to compute the Residue at z=z0. The function, fun, is assumed to return a result of the same shape and size as its input, *z*.

step: float, complex, array-like or StepGenerator object, optional
Defines the spacing used in the approximation. Default is CStepGenerator(base_step=step, **options)

method
[{'above', 'below'}] defines if the limit is taken from *above* or *below*

order: positive scalar integer, optional.
defines the order of approximation used to find the specified limit. The order must be member of [1 2 3 4 5 6 7 8]. 4 is a good compromise.

pole_order
[scalar integer] specifies the order of the pole at z0.

full_output: bool
If true return additional info.

options:
options to pass on to CStepGenerator

Returns

res_fz: array like
estimated residue, i.e., limit of f(z)*(z-z0)**pole_order as z –> z0 When the residue is estimated as approximately zero,

the wrong order pole may have been specified.

info: namedtuple,
Only given if full_output is True and contains the following:

error estimate: ndarray
95 % uncertainty estimate around the residue, such that abs(res_fz - lim z->z0 f(z)*(z-z0)**pole_order) < error_estimate Large uncertainties here suggest that the wrong order pole was specified for f(z0).

final_step: ndarray
final step used in approximation

Notes

Residue computes the residue of a given function at a simple first order pole, or at a second order pole.

The methods used by residue are polynomial extrapolants, which also yield an error estimate. The user can specify the method order, as well as the order of the pole.

z0 - scalar point at which to compute the residue. z0 may be
real or complex.

See the document DERIVEST.pdf for more explanation of the algorithms behind the parameters of Residue. In most cases, the user should never need to specify anything other than possibly the PoleOrder.

Examples

A first order pole at z = 0

```
>>> import numpy as np
>>> from numdifftools.limits import Residue
>>> def f(z): return -1./(np.expm1(2*z))
>>> res_f, info = Residue(f, full_output=True)(0)
>>> np.allclose(res_f, -0.5)
True
>>> info.error_estimate < 1e-14
True
```

A second order pole around z = 0 and z = pi >>> def h(z): return 1.0/np.sin(z)**2 >>> res_h, info = Residue(h, full_output=True, pole_order=2)([0, np.pi]) >>> np.allclose(res_h, 1) True >>> (info.error_estimate < 1e-10).all() True

5.2.7 numdifftools.multicomplex module

Created on 22. apr. 2015

@author: pab

5.2.7.1 References

A methodology for robust optimization of low-thrust trajectories in multi-body environments Gregory Lantoine (2010) Phd thesis, Georgia Institute of Technology

Using multicomplex variables for automatic computation of high-order derivatives Gregory Lantoine, Ryan P. Russell , and Thierry Dargent ACM Transactions on Mathematical Software, Vol. 38, No. 3, Article 16, April 2012, 21 pages, http://doi.acm.org/10.1145/2168773.2168774

Bicomplex Numbers and Their Elementary Functions M.E. Luna-Elizarraras, M. Shapiro, D.C. Struppa1, A. Vajiac (2012) CUBO A Mathematical Journal Vol. 14, No 2, (61-80). June 2012.

Computation of higher-order derivatives using the multi-complex step method Adriaen Verheyleweghen, (2014) Project report, NTNU

class Bicomplex(*z1*, *z2*)

Bases: `object`[62]

Creates an instance of a Bicomplex object. zeta = z1 + j*z2, where z1 and z2 are complex numbers.

arccos()

arccosh()

arcsin()

arcsinh()

arctan()

arctanh()

arg_c()

arg_c1p()

static asarray(*other*)

conjugate()

cos()

cosh()

cot()

coth()

csc()

csch()

dot(*other*)

exp()

exp2()

expm1()

flat(*index*)

property imag

property imag1

property imag12

property imag2

log()

log10()

log1p()

log2()

logaddexp(*other*)

logaddexp2(*other*)

static mat2bicomp(*arr*)

mod_c()

Complex modulus

norm()

property real

sec()

sech()

property shape

sin()

sinh()

property size

sqrt()

tan()

tanh()

z1

z2

c_abs(*z*)

c_atan2(*x*, *y*)

c_max(*x*, *y*)

c_min(*x*, *y*)

[62] https://docs.python.org/3.7/library/functions.html#object

5.2.8 numdifftools.nd_algopy module

5.2.8.1 Numdifftools.nd_algopy

This module provide an easy to use interface to derivatives calculated with AlgoPy. Algopy stands for Algorithmic Differentiation in Python.

The purpose of AlgoPy is the evaluation of higher-order derivatives in the forward and reverse mode of Algorithmic Differentiation (AD) of functions that are implemented as Python programs. Particular focus are functions that contain numerical linear algebra functions as they often appear in statistically motivated functions. The intended use of AlgoPy is for easy prototyping at reasonable execution speeds. More precisely, for a typical program a directional derivative takes order 10 times as much time as time as the function evaluation. This is approximately also true for the gradient.

5.2.8.2 Algoritmic differentiation

Algorithmic differentiation (AD) is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

Algorithmic differentiation is not:

Symbolic differentiation, nor Numerical differentiation (the method of finite differences). These classical methods run into problems: symbolic differentiation leads to inefficient code (unless carefully done) and faces the difficulty of converting a computer program into a single expression, while numerical differentiation can introduce round-off errors in the discretization process and cancellation. Both classical methods have problems with calculating higher derivatives, where the complexity and errors increase. Finally, both classical methods are slow at computing the partial derivatives of a function with respect to many inputs, as is needed for gradient-based optimization algorithms. Algoritmic differentiation solves all of these problems.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

https://pythonhosted.org/algopy/index.html

`class Derivative`(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Bases: `_Derivative`

Calculate n-th derivative with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

n: int, optional
Order of the derivative.

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

der: ndarray
array of derivatives

See also:

Gradient **(page 118)**
Hessdiag **(page 120)**
Hessian **(page 121)**
Jacobian **(page 123)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

1'st and 2'nd derivative of exp(x), at x == 1

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> fd = nda.Derivative(np.exp)               # 1'st derivative
>>> np.allclose(fd(1), 2.718281828459045)
True
>>> fd5 = nda.Derivative(np.exp, n=5)          # 5'th derivative
>>> np.allclose(fd5(1), 2.718281828459045)
True
```

1'st derivative of x^3+x^4, at x = [0,1]

```
>>> fun = lambda x: x**3 + x**4
>>> fd3 = nda.Derivative(fun)
>>> np.allclose(fd3([0,1]), [ 0.,  7.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

class Gradient(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Bases: _Derivative

Calculate Gradient with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

grad: array
gradient

See also:

Derivative **(page 117)**
Jacobian **(page 123)**
Hessdiag **(page 120)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> fun = lambda x: np.sum(x**2)
>>> df = nda.Gradient(fun, method='reverse')
>>> np.allclose(df([1,2,3]), [ 2.,  4.,  6.])
True
```

#At [x,y] = [1,1], compute the numerical gradient #of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nda.Gradient(z)
>>> grad2 = dz([1, 1])
>>> np.allclose(grad2, [ 3.71828183,  1.71828183])
True
```

#At the global minimizer (1,1) of the Rosenbrock function, #compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> rd = nda.Gradient(rosen)
>>> grad3 = rd([1,1])
>>> np.allclose(grad3, [ 0.,  0.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

class Hessdiag(*f*, *method='forward'*, *full_output=False*)

Bases: *Hessian* (page 121)

Calculate Hessian diagonal with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

hessdiag
[ndarray] Hessian diagonal array of partial second order derivatives.

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Jacobian **(page 123)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nda.Hessdiag(rosen)
>>> h = Hfun([1, 1]) #  h =[ 842, 210]
>>> np.allclose(h, [ 842.,  210.])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nda.Hessdiag(fun)
>>> h2 = Hfun2([0, 0]) # h2 = [-1, -1]
>>> np.allclose(h2, [-1., -1.])
True
```

```
>>> Hfun3 = nda.Hessdiag(fun, method='reverse')
>>> h3 = Hfun3([0, 0]) # h2 = [-1, -1];
>>> np.allclose(h3, [-1., -1.])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

class Hessian(*f*, *method='forward'*, *full_output=False*)

Bases: _Derivative

Calculate Hessian with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

hess
[ndarray] array of partial second derivatives, Hessian

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Jacobian **(page 123)**
Hessdiag **(page 120)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hf = nda.Hessian(rosen)
>>> h = Hf([1, 1]) #  h =[ 842 -420; -420, 210];
>>> np.allclose(h, [[ 842., -420.],
...                 [-420.,  210.]])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nda.Hessian(fun)
>>> h2 = Hfun2([0, 0]) # h2 = [-1 1; 1 -1]
>>> np.allclose(h2, [[-1.,  1.],
...                  [ 1., -1.]])
True
```

```
>>> Hfun3 = nda.Hessian(fun, method='reverse')
>>> h3 = Hfun3([0, 0]) # h2 = [-1, 1; 1, -1];
>>> np.allclose(h3, [[-1.,  1.],
...                  [ 1., -1.]])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

class Jacobian(*fun*, *n=1*, *method='forward'*, *full_output=False*)

Bases: *Gradient* (page 118)

Calculate Jacobian with Algorithmic Differentiation method

Parameters

fun: function
function of one array fun(x, **args*, ***kwds*)

method: string, optional {'forward', 'reverse'}
defines method used in the approximation

Returns

jacob: array
Jacobian

See also:

Derivative **(page 117)**
Gradient **(page 118)**
Hessdiag **(page 120)**
Hessian **(page 121)**

Notes

Algorithmic differentiation is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

References

Sebastian F. Walter and Lutz Lehmann 2013, "Algorithmic differentiation in Python with AlgoPy", in Journal of Computational Science, vol 4, no 5, pp 334 - 344, http://www.sciencedirect.com/science/article/pii/S1877750311001013

https://en.wikipedia.org/wiki/Automatic_differentiation

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
```

Jfun = nda.Jacobian(fun) # Todo: This does not work Jfun([1,2,0.75]).T # should be numerically zero array([[0., 0., 0., 0., 0., 0., 0., 0., 0., 0.],

[0., 0., 0., 0., 0., 0., 0., 0., 0., 0.], [0., 0., 0., 0., 0., 0., 0., 0., 0., 0.]])

```
>>> Jfun2 = nda.Jacobian(fun, method='reverse')
>>> res = Jfun2([1,2,0.75]).T # should be numerically zero
>>> np.allclose(res,
...                [[ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.],
...                 [ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.],
...                 [ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.]])
True
```

```
>>> f2 = lambda x : x[0]*x[1]*x[2]**2
>>> Jfun2 = nda.Jacobian(f2)
>>> np.allclose(Jfun2([1., 2., 3.]), [[ 18., 9., 12.]])
True
```

```
>>> Jfun21 = nda.Jacobian(f2, method='reverse')
>>> np.allclose(Jfun21([1., 2., 3.]), [[ 18., 9., 12.]])
True
```

```
>>> def fun3(x):
...     n = int(np.prod(np.shape(x[0])))
...     out = nda.algopy.zeros((2, n), dtype=x)
...     out[0] = x[0]*x[1]*x[2]**2
...     out[1] = x[0]*x[1]*x[2]
...     return out
>>> Jfun3 = nda.Jacobian(fun3)
```

```
>>> np.allclose(Jfun3([1., 2., 3.]), [[[18., 9., 12.]], [[6., 3., 2.]]])
True
>>> np.allclose(Jfun3([4., 5., 6.]), [[[180., 144., 240.]],
...                                   [[30., 24., 20.]]])
True
>>> np.allclose(Jfun3(np.array([[1.,2.,3.], [4., 5., 6.]]).T),
...             [[[18.,    0.,    9.,    0.,   12.,    0.],
...               [0.,  180.,    0.,  144.,    0.,  240.]],
...              [[6.,    0.,    3.,    0.,    2.,    0.],
...               [0.,   30.,    0.,   24.,    0.,   20.]]])
True
```

Methods

__call__: callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function *fun*. kwds: dict Keyword arguments for function *fun*.

class Taylor(*fun*, *n=1*)

Bases: object[63]

Return Taylor coefficients of function using algorithmic differentiation

Parameters

fun: callable
function to differentiate

z0: real or complex array
at which to evaluate the derivatives

n: scalar integer, default 1
Number of taylor coefficents to compute.

Returns

coefs: ndarray
array of taylor coefficents

Examples

Compute the first 6 taylor coefficients 1 + 2*z + 3*z**2 expanded round z0 = 0:

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> c = nda.Taylor(lambda x: 1+2*x+3*x**2, n=6)(z0=0)
>>> np.allclose(c, [1, 2, 3, 0, 0, 0])
True
```

directionaldiff(*f*, *x0*, *vec*, ***options*)

Return directional derivative of a function of n variables

Parameters

fun: callable
analytical function to differentiate.

x0: array
vector location at which to differentiate fun. If x0 is an nxm array, then fun is assumed to be a function of n*m variables.

vec: array
vector defining the line along which to take the derivative. It should be the same size as x0, but need not be a vector of unit length.

****options:**
optional arguments to pass on to Derivative.

Returns

dder: scalar
estimate of the first derivative of fun in the specified direction.

See also:

Derivative **(page 117)**
Gradient **(page 118)**

Examples

At the global minimizer (1,1) of the Rosenbrock function, compute the directional derivative in the direction [1 2]

```
>>> import numpy as np
>>> import numdifftools.nd_algopy as nda
>>> vec = np.r_[1, 2]
>>> rosen = lambda x: (1-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> dd = nda.directionaldiff(rosen, [1, 1], vec)
```

(continues on next page)

[63] https://docs.python.org/3.7/library/functions.html#object

(continued from previous page)

```
>>> np.allclose(dd, 0)
True
```

5.2.9 numdifftools.nd_scipy module

class Gradient(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Bases: *Jacobian* (page 126)

Calculate Gradient with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
[{'central', 'complex', 'forward'}] defines the method used in the approximation.

See also:

Hessian, *Jacobian* (page 126)

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_scipy as nd
>>> fun = lambda x: np.sum(x**2)
>>> dfun = nd.Gradient(fun)
>>> np.allclose(dfun([1,2,3]), [ 2.,  4.,  6.])
True
```

At [x,y] = [1,1], compute the numerical gradient # of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nd.Gradient(z)
>>> grad2 = dz([1, 1])
>>> np.allclose(grad2, [ 3.71828183,  1.71828183])
True
```

At the global minimizer (1,1) of the Rosenbrock function, # compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> rd = nd.Gradient(rosen)
>>> grad3 = rd([1,1])
>>> np.allclose(grad3,[0, 0], atol=1e-7)
True
```

class Jacobian(*fun*, *step=None*, *method='central'*, *order=2*, *bounds=(-inf, inf)*, *sparsity=None*)

Bases: _Common

Calculate Jacobian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
[{'central', 'complex', 'forward'}] defines the method used in the approximation.

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_scipy as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape, (10,))
True
>>> dfun = nd.Jacobian(fun)
>>> np.allclose(dfun([1, 2, 0.75]), np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> dfun2 = nd.Jacobian(fun2)
>>> np.allclose(dfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
```

TODO: The following does not work: der3 = nd.Jacobian(fun3)([1., 2., 3.]) np.allclose(der3, … [[18., 9., 12.], [6., 3., 2.]]) True np.allclose(nd.Jacobian(fun3)([4., 5., 6.]), … [[180., 144., 240.], [30., 24., 20.]]) True

np.allclose(nd.Jacobian(fun3)(np.array([[1.,2.,3.], [4., 5., 6.]]).T), … [[[18., 180.], … [9., 144.], … [12., 240.]], … [[6., 30.], … [3., 24.], … [2., 20.]]]) True

5.2.10 numdifftools.nd_statsmodels module

5.2.10.1 Numdifftools.nd_statsmodels

This module provides an easy to use interface to derivatives calculated with statsmodels.numdiff.

class Gradient(*fun*, *step=None*, *method='central'*, *order=None*)

Bases: *Jacobian* (page 129)

Calculate Gradient with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
: [float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
: [{'central', 'complex', 'forward', 'backward'}] defines the method used in the approximation.

See also:

Hessian **(page 128),** *Jacobian* **(page 129)**

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_statsmodels as nd
>>> fun = lambda x: np.sum(x**2)
>>> dfun = nd.Gradient(fun)
>>> np.allclose(dfun([1,2,3]), [ 2.,  4.,  6.])
True
```

At [x,y] = [1,1], compute the numerical gradient # of the function sin(x-y) + y*exp(x)

```
>>> sin = np.sin; exp = np.exp
>>> z = lambda xy: sin(xy[0]-xy[1]) + xy[1]*exp(xy[0])
>>> dz = nd.Gradient(z)
>>> grad2 = dz([1, 1])
>>> np.allclose(grad2, [ 3.71828183,  1.71828183])
True
```

At the global minimizer (1,1) of the Rosenbrock function, # compute the gradient. It should be essentially zero.

```
>>> rosen = lambda x : (1-x[0])**2 + 105.*(x[1]-x[0]**2)**2
>>> rd = nd.Gradient(rosen)
>>> grad3 = rd([1,1])
>>> np.allclose(grad3,[0, 0])
True
```

class Hessian(*fun*, *step=None*, *method='central'*, *order=None*)

Bases: _Common

Calculate Hessian with finite difference approximation

Parameters

fun
: [function] function of one array fun(x, **args*, ***kwds*)

step
: [float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS**(1/3) for method==`forward`, *complex* or *central2* x * _EPS**(1/4) for method==`central`.

method
: [{'central', 'complex', 'forward', 'backward'}] defines the method used in the approximation.

See also:

Jacobian **(page 129),** *Gradient* **(page 127)**

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_statsmodels as nd
```

Rosenbrock function, minimized at [1,1]

```
>>> rosen = lambda x : (1.-x[0])**2 + 105*(x[1]-x[0]**2)**2
>>> Hfun = nd.Hessian(rosen)
>>> h = Hfun([1, 1])
>>> np.allclose(h, [[ 842., -420.], [-420.,  210.]])
True
```

cos(x-y), at (0,0)

```
>>> cos = np.cos
>>> fun = lambda xy : cos(xy[0]-xy[1])
>>> Hfun2 = nd.Hessian(fun)
>>> h2 = Hfun2([0, 0])
>>> np.allclose(h2, [[-1.,  1.], [ 1., -1.]])
True
```

property n

class Jacobian(*fun*, *step=None*, *method='central'*, *order=None*)

Bases: _Common

Calculate Jacobian with finite difference approximation

Parameters

fun
[function] function of one array fun(x, **args*, ***kwds*)

step
[float, optional] Stepsize, if None, optimal stepsize is used, i.e., x * _EPS for method==`complex` x * _EPS**(1/2) for method==`forward` x * _EPS**(1/3) for method==`central`.

method
[{'central', 'complex', 'forward', 'backward'}] defines the method used in the approximation.

Examples

```
>>> import numpy as np
>>> import numdifftools.nd_statsmodels as nd
```

#(nonlinear least squares)

```
>>> xdata = np.arange(0,1,0.1)
>>> ydata = 1+2*np.exp(0.75*xdata)
>>> fun = lambda c: (c[0]+c[1]*np.exp(c[2]*xdata) - ydata)**2
>>> np.allclose(fun([1, 2, 0.75]).shape, (10,))
True
>>> dfun = nd.Jacobian(fun)
>>> np.allclose(dfun([1, 2, 0.75]), np.zeros((10,3)))
True
```

```
>>> fun2 = lambda x : x[0]*x[1]*x[2]**2
>>> dfun2 = nd.Jacobian(fun2)
>>> np.allclose(dfun2([1.,2.,3.]), [[18., 9., 12.]])
True
```

```
>>> fun3 = lambda x : np.vstack((x[0]*x[1]*x[2]**2, x[0]*x[1]*x[2]))
>>> np.allclose(nd.Jacobian(fun3)([1., 2., 3.]), [[[18.], [9.], [12.]], [[6.],␣
↪[3.], [2.]]])
True
>>> np.allclose(nd.Jacobian(fun3)([4., 5., 6.]),
...             [[[180.], [144.], [240.]], [[30.], [24.], [20.]]])
True
```

```
>>> np.allclose(nd.Jacobian(fun3)(np.array([[1.,2.,3.], [4., 5., 6.]]).T),
...             [[[  18.,  180.],
...               [   9.,  144.],
...               [  12.,  240.]],
...              [[   6.,   30.],
...               [   3.,   24.],
...               [   2.,   20.]]])
True
```

approx_fprime(*x*, *f*, *epsilon=None*, *args=()*, *kwargs=None*, *centered=True*)

Gradient of function, or Jacobian if function fun returns 1d array

Parameters

x
[array] parameters at which the derivative is evaluated

fun
[function] *fun(*((x,)+args), **kwargs)* returning either one value or 1d array

epsilon
[float, optional] Stepsize, if None, optimal stepsize is used. This is _EPS**(1/2)*x for *centered* == False and _EPS**(1/3)*x for *centered* == True.

args
[tuple] Tuple of additional arguments for function *fun*.

kwargs
[dict] Dictionary of additional keyword arguments for function *fun*.

centered
[bool] Whether central difference should be returned. If not, does forward differencing.

Returns

grad
[array] gradient or Jacobian

Notes

If fun returns a 1d array, it returns a Jacobian. If a 2d array is returned by fun (e.g., with a value for each observation), it returns a 3d array with the Jacobian of each observation with shape xk x nobs x xk. I.e., the Jacobian of the first observation would be [:, 0, :]

approx_fprime_cs(*x*, *f*, *epsilon=None*, *args=()*, *kwargs=None*)

Calculate gradient or Jacobian with complex step derivative approximation

Parameters

x
[array] parameters at which the derivative is evaluated

f
[function] *f(*(x,)+args), **kwargs)* returning either one value or 1d array

epsilon
[float, optional] Stepsize, if None, optimal stepsize is used. Optimal step-size is EPS*x. See note.

args
[tuple] Tuple of additional arguments for function *f*.

kwargs
[dict] Dictionary of additional keyword arguments for function *f*.

Returns

partials
[ndarray] array of partial derivatives, Gradient or Jacobian

Notes

The complex-step derivative has truncation error O(epsilon**2), so truncation error can be eliminated by choosing epsilon to be very small. The complex-step derivative avoids the problem of round-off error with small epsilon because there is no subtraction.

5.2.11 numdifftools.step_generators module

Step generators module

class BasicMaxStepGenerator(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Bases: object[64]

Generates a sequence of steps of decreasing magnitude

where
steps = base_step * step_ratio ** (-i + offset)

for i=0, 1,.., num_steps-1.

Parameters

base_step
[float, array-like.] Defines the start step, i.e., maximum step

step_ratio
[real scalar.] Ratio between sequential steps generated. Note: Ratio > 1

num_steps
[scalar integer.] defines number of steps generated.

offset
[real scalar, optional, default 0] offset to the base step

Examples

```
>>> from numdifftools.step_generators import BasicMaxStepGenerator
>>> step_gen = BasicMaxStepGenerator(base_step=2.0, step_ratio=2,
...                                  num_steps=4)
>>> [s for s in step_gen()]
[2.0, 1.0, 0.5, 0.25]
```

class BasicMinStepGenerator(*base_step*, *step_ratio*, *num_steps*, *offset=0*)

Bases: *BasicMaxStepGenerator* (page 131)

Generates a sequence of steps of decreasing magnitude

where

steps = base_step * step_ratio ** (i + offset), i=num_steps-1,... 1, 0.

Parameters

base_step
[float, array-like.] Defines the end step, i.e., minimum step

step_ratio
[real scalar.] Ratio between sequential steps generated. Note: Ratio > 1

num_steps
[scalar integer.] defines number of steps generated.

offset
[real scalar, optional, default 0] offset to the base step

Examples

```
>>> from numdifftools.step_generators import BasicMinStepGenerator
>>> step_gen = BasicMinStepGenerator(base_step=0.25, step_ratio=2,
...                                  num_steps=4)
>>> [s for s in step_gen()]
[2.0, 1.0, 0.5, 0.25]
```

class MaxStepGenerator(*base_step=2.0*, *step_ratio=None*, *num_steps=15*, *step_nom=None*, *offset=0*, *num_extrap=9*, *use_exact_steps=False*, *check_num_steps=True*, *scale=500*)

Bases: *MinStepGenerator* (page 133)

Generates a sequence of steps

where

steps = step_nom * base_step * step_ratio ** (-i + offset)

for i = 0, 1, ..., num_steps-1.

Parameters

base_step
[float, array-like, default 2.0] Defines the maximum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 2 or 1.6] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

[64] https://docs.python.org/3.7/library/functions.html#object

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, default 500] scale used in base step.

`class MinStepGenerator`(*base_step=None*, *step_ratio=None*, *num_steps=None*, *step_nom=None*, *offset=0*, *num_extrap=0*, *use_exact_steps=True*, *check_num_steps=True*, *scale=None*)

Bases: `object`[65]

Generates a sequence of steps

where
steps = step_nom * base_step * step_ratio ** (i + offset)

for i = num_steps-1,... 1, 0.

Parameters

base_step
[float, array-like, optional] Defines the minimum step, if None, the value is set to EPS**(1/scale)

step_ratio
[real scalar, optional, default 2] Ratio between sequential steps generated. Note: Ratio > 1 If None then step_ratio is 2 for n=1 otherwise step_ratio is 1.6

num_steps
[scalar integer, optional, default min_num_steps + num_extrap] defines number of steps generated. It should be larger than min_num_steps = (n + order - 1) / fact where fact is 1, 2 or 4 depending on differentiation method used.

step_nom
[default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at runtime through the __call__ method.

offset
[real scalar, optional, default 0] offset to the base step

num_extrap
[scalar integer, default 0] number of points used for extrapolation

check_num_steps
[boolean, default True] If True make sure num_steps is larger than the minimum required steps.

use_exact_steps
[boolean, default True] If true make sure exact steps are generated

scale
[real scalar, optional] scale used in base step. If not None it will override the default computed with the default_scale function.

property base_step
Base step defines the minimum or maximum step when offset==0.

property min_num_steps
Minimum number of steps required given the differentiation method and order.

property num_steps
Defines number of steps generated

property scale
Scale used in base step.

step_generator_function(*x*, *method='forward'*, *n=1*, *order=2*)
Step generator function

property step_nom
Nominal step

property step_ratio
Ratio between sequential steps generated

default_scale(*method='forward'*, *n=1*, *order=2*)
Returns good scale for MinStepGenerator

get_base_step(*scale*)
Return base_step = EPS ** (1. / scale)

get_nominal_step(*x=None*)
Return nominal step

make_exact(*h*)
Make sure h is an exact representable number

This is important when calculating numerical derivatives and is accomplished by adding 1.0 and then subtracting 1.0.

[65] https://docs.python.org/3.7/library/functions.html#object

APPENDIX

A

CHANGELOG

A.1 Version 0.9.41 Nov 10, 2022

Fabian Joswig (5):

- ci: execute test action only on push to master and on pull requests.
- ci: test requirements added to ci workflow.
- ci: first version of github actions ci added.
- fix: import from from scipy.ndimage.filters replaced by from scipy.ndimage
- fix: np.info(float).machar.tiny replaced by np.info(float).tiny

Jonas Eschle (6):

- Drop Python 3.6
- Remove Python 2.7, 3.6 from appveyor CI
- Update .travis.yml
- Update setup.cfg
- Update .travis.yml
- Update to Python310

Per A Brodtkorb (19):

- Commented out deprecated pep8ignore and pep8maxlinelength in setup.cfg
- Fixed issue #59: numpy deprecation warning on machar.tiny
- Deleted obsolete travis_install.sh
- Replaced deprecated *np.MachAr().eps* (NumPy 1.22) with np.finfo(float).eps in test_multicomplex.py
- Added requirements.tests.txt
- Updated .github/workflows/test.yml to use requirements.tests.txt
- Removed obsolete .travis.yml and appveyor.yml.
- Github-actions are now used instead.
- Replaced appveyor badge and travis badge with github-actions badge in README.rst, info.py and index.rst
- Removed python 2.7 from classifiers in setup.cfg
- Updated .travis.yml
- Fixed doctest so they don't crash on travis: Replaced "# doctest + SKIP" with "# doctest: +SKIP" in docstrings.
- Updated download badge in README.rst and info.py

- Updated test_img in README.rst
- Updated tests_img path for travis.
- Added "# doctest + SKIP" to doctest string in info.py
- Replaced "version|" with "release|" in docs/index.rst
- Added matplotlib to requirements.txt Removed failing python 3.8 from appveyor.yml

Per A. Brodtkorb (4):

- Merge pull request #65 from fjosw/feat/github_actions_ci
- Merge pull request #66 from jonas-eschle/patch-1
- Merge pull request #60 from peendebak/performance/percentile
- Merge pull request #63 from fjosw/feat/numpy_deprecation

Pieter Eendebak (2):

- workaround for known issue with np.nanpercentile
- improve performance by combining percentile calculations

A.2 Version 0.9.40 Jun 2, 2021

Per A Brodtkorb (109):

- Replaced python 3.5 with 3.9 in .travis.yml
- Removed python 3.5 from appveyor.yml
- Added bibtex_bibfiles = ... to docs/conf.py
- **Fixed doctest failures in**
  - docs/src/numerical/derivest.rst
  - docs/tutorials/getting_started.rst
  - numdifftools.core.py
  - numdifftools.limits.py
  - numdifftools.nd_algopy.py
  - numdifftools.nd_scipy.py
  - numdifftools.nd_statsmodels.py
- Insulated import of click in a if __name__ ==’__main__’ clause.
- Added activate to appveyor.yml
- Added https://mathworld.wolfram.com/WynnsEpsilonMethod.html reference for the Epsilon algorithm in extrapolation.py.
- Disabled the restriction that n must be one in LogJacobianRule
- Added complex_even and central_even methods to the JacobianDifferenceFunctions
- Updated documentation of Derivative in core.py
- Updated documentation of Richardson.
- Removed obsolete tests from test_nd_scipy.py
- Fixed a bug in TestJacobian.test_scalar_to_vector in test_nd_scipy.py for method=”complex’
- Refactored code from core.py to finite_difference.py

- Added LogJacobianRule, LogHessdiagRule, LogHessianRule to finite_difference.py
- Fixed a bug in Richardson._estimate_error: Complex rule resulted wrongly in complex error values.
- Added netlib.org/quadpack reference.
- Updated Dea to conform with Quadpack
- Replaced reference to Brezinski with refs to Quadpack.
- Reduced cyclomatic complexity in Dea in extrapolation.py
- Removed commented out code in profile_numdifftools.py
- Updated pycodestyle ignore section in setup.cfg
- Removed commented out code in run_benchmark.py Made get_nominal_step continous as function of x
- Made datetime call python 2.7 compatible in run_benchmark.py
- Simplified the Derivative._step_generator function in core.py.
- Made plots generated from run_benchmark.py prettier.
- step_ratio in the step generators by default 2 for n=1 and 1.6 otherwise in step_generators.py
- Fixed failing doctests in core.py and nd_statsmodels.py
- Added doctests to setup.cfg.
- Reordered imports in test_example_functions.py
- Fixed .travis.yml so that he file paths in coverage.xml is discoverable under the sonar.sources folder. The problem is that SonarQube is analysing the checked-out source code (in src/numdifftools) but the actual unit tests and coverage.py is run against the installed code (in build/lib/numdifftools). Thus the absolute files paths to the installed
- Removed commented code from test_numdifftools.py
- Run only coverage xml when python version is 3.7
- Updated .travis.yml Removed commented out code from extrapolation.py and nd_statsmodels.py
- Finalized the moved of XXXDifferencdFunctions from core.py to finite_difference.py
- Added missing docstring for default_scale function in step_generators.py.
- Removed unused import of itertools in _find_default_scale.py.
- Changed default scale from 1.35 to 1.06 for complex/multicomplex methods when n=1
- Added richardson_demo to extrapolation.py Simplified EpsAlg class in extrapolation.py
- Corrected a small error for dea3: Now dea3 and Dea(limexp=3) gives the same result!
- Added python 3.8 to appveyor.yml Added python 3.9 to setup.cfg
- Fixed reference to how-to/index
- Added doctest configuration to docs.conf.py
- Fixes issue #50 by adding function value f(x) to the info.f_value.
- Updated README.rst
- Added @UnusedVariable here and there.
- Silence warnings in Hessian by adding __init__ that set the correct order given the method.
- Updated the Richardson._r_matrix method to generate complex matrix when step_ratio is complex.
- Fixed profile_hessian in profile_numdifftools.py so it works again.
- Added with np.errstate(all='ignore') to test_derivative_on_sinh and test_scalar_to_vector in test_nd_algopy.py to silence warnings.

- Changed citation style to alpha.
- Replaced bibliography.rst with refs1.bib and zreferences.rst
- Removed badges for latex
- Changed sonar addon token
- Added CC_TEST_REPORTER_ID
- Fixed a typo in docs/numdifftools.rst
- Added docs/make.bat
- Removed python 2.7 from .travis.yml
- Moved test_requires from setup.cfg to setup.py
- Added Latex to setup.py
- Changed default radius to 0.0059 which appears to cause less failures in Taylor in fornberg.py.
- Updated MANIFEST.in
- Fixes issue #49 : Dimension of Jacobian of vector valued function (length n) with scalar input should be n X 1
- Updated build_package.py
- Attempt to silence divide by zero and invalid warnings.
- Fix issue#52: Gradient tries to apply squeeze to the output tuple containing both the result and the full_output object.
- Made docstring a rawdocstring since it contains slashes.
- Added "# pylint: disable=unused-argument" in appropriate places.
- API change: replaced "python setup.py doctests" with "python setup.py doctest"
- Removed unused imports
- Fixed a bug in test_low_order_derivative_on_example_functions: Same variable (i) was used both in the outer and inner loop.
- Updated badge for pypi and documentation of fornberg.py
- Fixed failing tests.
- Updated docs + added a test
- Added "python -m pip install –upgrade pytest" to appveyor.yml due to a package conflict on python2.7 32 bit
- Added - "python -m pip install –upgrade setuptools" in appveyor.yml to avoid build error.
- Try "python setup.py bdist_wheel" and "pip install numdifftools –find-links=dist" in appveyor.yml
- Put qoutes on "python -m pip install –upgrade pip" in appveyor.yml
- **Changed "python setup.py install" to**
  - python setup.py bdist_wheel"
  - pip install numdifftools –find-links=dist
- Added "pip install –upgrade pip" to appveyor.yml
- Updated the detailed package documentation.
- Added missing pytest-pep8 to install
- Updated badge + appveyor.yml
- ongoing work to harmonize the the output from approx_fprime and approx_fprime_cs

- Added Taylor class to nd_algopy.py Fixed a bug in _get_best_taylor_coefficient in fornberg.py
- Updated references Added test_mod_c function to test_multicomplex.py
- Fixed a typo.
- Removed –strict-markers
- Fixed issue #39 TypeError: unsupported operand type(s) for /: 'float' and 'Bicomplex'
- Fixed a typo in the documentation. Closing issue #51
- Added separate test for nd_scipy.
- added skip on tests if LineProfiler is not installed.
- Removed obsolete centered argument from call to approx_hess1 + pep8
- Move Jacobian._increment method to _JacobianDifferenceFunctions
- step_nom was unused in CStepGenerator.__init__ Added pytest.markers.slow in to setup.cfg
- Made two tests more forgiving in order to avoid failure on travis.
- Renamed nominal_step and base_step to get_nominal_step and get_base_step, respectively.
- Removed obsolete import of example from hypothesis
- Updated testing
- Updated coverage call: coverage run -m py.test src/numdifftools/tests
- Delete obsolete conftest.py

A.3 Version 0.9.39 Jun 10, 2019

Robert Parini (1):

- Fix issue #43: numpy future warning

A.4 Version 0.9.38 Jun 10, 2019

Andrew Nelson (1):

- MAINT: special.factorial instead of misc.factorial

Dougal J. Sutherland (1):

- include LICENSE.txt in distributions

Per A Brodtkorb (140):

- Adjusted runtime for hypothesis tests to avoid failure and fixed pep8 failures.
- Fixed a bug in setup.cfg
- Replaced valarray function with numpy.full in step_generators.py
- Added try except on import of algopy
- Updated the badges used in the README.rst
- Replaced numpy.testing.Tester with pytest.
- Removed dependence on pyscaffold.
- Simplified setup.py and setup.cfg
- Updated .travis.yml configuration.

- Reorganized the documentation.
- Ongoing work to simplify the classes.
- Replaced unittest with pytest.
- Added finite_difference.py
- replaced , with .
- Reverted to coverage=4.3.4
- New attempt
- Fixed conflicting import
- Missing import of EPS
- Added missing FD_RULES = { }
- Removed pinned coverage, removed dependence on pyscaffold
- Updated .travis.yml and .appveyor.yml
- Replaced conda channel omnia with conda-forge
- Removed commented out code. Set pyqt=5 in appveyor.yml
- Updated codeclimate checks
- Dropped support for python 3.3 and 3.4. Added support for python 3.6, 3.7
- Simplified code.
- Pinned IPython==5.0 in order to make the testserver not crash.
- Added line_profiler to appveyor.yml
- Removed line_profiler from requirements.txt
- Fix issue #37: Unable to install on Python 2.7
- Added method='backward' to nd_statsmodels.py
- Skip test_profile_numdifftools_profile_hessian and TestDoProfile
- Added missing import of warnings
- Added tests for the scripts from profile_numdifftools.py, _find_default_scale.py and run_benchmark.py.
- Added reason to unittest.skipIf
- Added line_profiler to requirements.
- misssing import of warnings fixed.
- Renamed test so it comes last, because I suspect this test mess up the coverage stats.
- Reordered the tests.
- Added more tests.
- Cleaned up _find_default_scale.py
- Removed link to depsy
- Reverted: install of cython and pip install setuptools
- Disabled sonar-scanner -X for python 3.5 because it crashes.
- Reverted [options.packages.find] to exclude tests again
- Added cython and reverted to pip install setuptools
- Updated sphinx to 1.6.7

- Try to install setuptools with conda instead.
- Added hypothesis and pytest to requirements.readthedocs.txt
- Set version of setuptools==37.0
- Added algopy, statsmodels and numpy to requirements.readthedocs.txt
- Restricted sphinx in the hope that the docs will be generated.
- Removed exclusion of tests/ directory from test coverage.
- Added dependencies into setup.cfg
- Readded six as dependency
- Refactored and removed commented out code.
- Fixed a bug in the docstring example: Made sure the shape passed on to zeros is an integer.
- Fixed c_abs so it works with algopy on python 3.6.
- Fixed flaky test and made it more robust.
- Fixed bug in .travis.yml
- Refactored the taylor function into the Taylor class in order to simplify the code.
- Fixed issue #35 and added tests
- Attempt to simplify complexity
- Made doctests more robust
- Updated project path
- Changed install of algopy
- Fixed small bugs
- Updated docstrings
- Changed Example and Reference to Examples and References in docstrings to comply with numpydoc-style.
- Renamed CHANGES.rst to CHANGELOG.rst
- Renamed source path
- Hack due to a bug in algopy or changed behaviour.
- Small fix.
- Try to reduce complexity
- Reduced cognitive complexity of min_num_steps
- Simplified code in Jacobian
- Merge branch 'master' of https://github.com/pbrod/numdifftools
- Fixed issue #34 Licence clarification.
- Locked coverage=4.3.4 due to a bug in coverage that cause code-climate test-reporter to fail.
- Added script for finding default scale
- updated from sonarcube to sonarcloud
- Made sure shape is an integer.
- Refactored make_step_generator into a step property
- Issue warning message to the user when setting the order to something different than 1 or 2 in Hessian.
- Updated example in Gradient.

- Reverted –timid option to coverage because it took too long time to run.
- Reverted –pep8 option
- pep8 + added –timid in .travis.yml coverage run in order to to increase missed coverage.
- Refactored taylor to reduce complexity
- No support for python 3.3. Added python 3.6
- Fixed a small bug and updated test.
- Removed unneccasarry perenthesis. Reduced the complexity of do_profile
- Made python3 compatible
- Removed assert False
- Made unittests more forgiving.
- updated doctest in nd_scipy.py and profiletools.py install line_profiler on travis
- Made python 3 compatible
- Updated tests
- Added test_profiletools.py and capture_stdout_and_stderr in testing.py
- Optimized numdifftools.core.py for speed: fd_rules are now only computed once.
- Only keeping html docs in the distribution.
- Added doctest and updated .pylintrc and requirements.txt
- Reduced time footprint on tests in the hope that it will pass on Travis CI.
- Prefer static methods over instance methods
- Better memory handling: This fixes issue #27
- Added statsmodels to requirements.txt
- Added nd_statsmodels.py
- Simplified input
- Merge branch 'master' of https://github.com/pbrod/numdifftools
- Updated link to the documentation.

Robert Parini (4):

- Avoid RuntimeWarning in _get_logn
- Allow fd_derivative to take complex valued functions

solarjoe (1):

- doc: added nd.directionaldiff example

A.5 Version 0.9.20, Jan 11, 2017

Per A Brodtkorb (1):

- Updated the author email address in order for twine to be able to upload to pypi.

A.6 Version 0.9.19, Jan 11, 2017

Per A Brodtkorb (1):

- Updated setup.py in a attempt to get upload to pypi working again.

A.7 Version 0.9.18, Jan 11, 2017

Per A Brodtkorb (38):

- Updated setup
- Added import statements in help header examples.
- Added more rigorous tests using hypothesis.
- Forced to use wxagg backend
- Moved import of matplotlib.pyplot to main in order to avoid import error on travis.
- Added fd_derivative function
- Updated references.
- Attempt to automate sonarcube analysis
- Added testcoverage to sonarqube and codeclimate
- Simplified code
- Added .pylintrc + pep8
- Major change in api: class member variable self.f changed to self.fun
- Fixes issue #25 (Jacobian broken since 0.9.15)

A.8 Version 0.9.17, Sep 8, 2016

Andrew Fowlie (1):

- Fix ReadTheDocs link as mentioned in #21

Per A Brodtkorb (79):

- Added test for MinMaxStepgenerator
- Removed obsolete docs from core.py
- Updated appveyor.yml
- Fixed sign in inverse matrix
- Simplified code
- Added appveyor badge + synchronised info.py with README.rst.
- Removed plot in help header
- Added Programming Language :: Python :: 3.5
- Simplified code
- Renamed bicomplex to Bicomplex
- Simplified example_functions.py
- **Moved MinStepGenerator, MaxStepGeneretor and MinMaxStepGenerator to step_generators.py**

    - Unified the step generators
    - Moved step_generator tests to test_step_generators.py
    - Major simplification of step_generators.py
- Removed duplicated code + pep8
- Moved fornberg_weights to fornberg.py + added taylor and derivative
- Fixed print statement
- Replace xrange with range
- Added examples + made computation more robust.
- Made 'backward' and alias for 'reverse' in nd_algopy.py
- Expanded the tests + added test_docstrings to testing.py
- Replace string interpolation with format()
- Removed obsolete parameter
- Smaller start radius for Fornberg method
- Simplified "n" and "order" properties
- Simplified default_scale
- Removed unecessary parenthesis and code.
- Fixed a bug in Dea + small refactorings.
- Added test for EpsAlg
- Avoid mutable default args and prefer static methods over instance-meth.
- Refactored to reduce cyclomatic complexity
- Changed some instance methods to static methods
- Renamed non-pythonic variable names
- Turned on xvfb (X Virtual Framebuffer) to imitate a display.
- Added extra test for Jacobian
- Replace lambda function with a def
- Removed unused import
- Added test for epsalg
- Fixed test_scalar_to_vector
- Updated test_docstrings

A.9 Version 0.9.15, May 10, 2016

Cody (2):

- Migrated % string formating
- Migrated % string formating

Per A Brodtkorb (28):

- Updated README.rst + setup.cfg
- Replaced instance methods with static methods +pep8
- Merge branch 'master' of https://github.com/pbrod/numdifftools

- Fixed a bug: replaced missing triple quote
- Added depsy badge
- added .checkignore for quantificode
- Added .codeclimate.yml
- Fixed failing tests
- Changed instance methods to static methods
- Made untyped exception handlers specific
- Replaced local function with a static method
- Simplified tests
- Removed duplicated code Simplified _Derivative._get_function_name
- exclude tests from testclimate
- Renamed test_functions.py to example_functions.py Added test_example_functions.py

Per A. Brodtkorb (2):

- Merge pull request #17 from pbrod/autofix/wrapped2_to3_fix
- Merge pull request #18 from pbrod/autofix/wrapped2_to3_fix-0

pbrod (17):

- updated conf.py
- added numpydoc>=0.5, sphinx_rtd_theme>=0.1.7 to setup_requires if sphinx
- updated setup.py
- added requirements.readthedocs.txt
- Updated README.rst with info about how to install it using conda in an anaconda package.
- updated conda install description
- Fixed number of arguments so it does not differs from overridden '_default_base_step' method
- Added codecov to .travis.yml
- Attempt to remove coverage of test-files
- Added directionaldiff function in order to calculate directional derivatives. Fixes issue #16. Also added supporting tests and examples to the documentation.
- Fixed isssue #19 multiple observations mishandled in Jacobian
- Moved rosen function into numdifftools.testing.py
- updated import of rosen function from numdifftools.testing
- Simplified code + pep8 + added TestResidue
- Updated readme.rst and replaced string interpolation with format()
- Cleaned Dea class + pep8
- Updated references for Wynn extrapolation method.

A.10 Version 0.9.14, November 10, 2015

pbrod (53):

- Updated documentation of setup.py
- Updated README.rst
- updated version
- Added more documentation
- Updated example
- Added .landscape.yml updated .coveragerc, .travis.yml
- Added coverageall to README.rst.
- updated docs/index.rst
- Removed unused code and added tests/test_extrapolation.py
- updated tests
- Added more tests
- Readded c_abs c_atan2
- Removed dependence on wheel, numpydoc>=0.5 and sphinx_rtd_theme>=0.1.7 (only needed for building documentation)
- updated conda path in .travis.yml
- added omnia channel to .travis.yml
- Added conda_recipe files Filtered out warnings in limits.py

A.11 Version 0.9.13, October 30, 2015

pbrod (21):

- Updated README.rst and CHANGES.rst.
- updated Limits.
- Made it possible to differentiate complex functions and allow zero'th order derivative.
- BUG: added missing derivative order, n to Gradient, Hessian, Jacobian.
- Made test more robust.
- Updated structure in setup according to pyscaffold version 2.4.2.
- Updated setup.cfg and deleted duplicate tests folder.
- removed unused code.
- Added appveyor.yml.
- Added required appveyor install scripts
- Fixed bug in appveyor.yml.
- added wheel to requirements.txt.
- updated appveyor.yml.
- Removed import matplotlib.

Justin Lecher (1):

- Fix min version for numpy.

kikocorreoso (1):

- fix some prints on run_benchmark.py to make it work with py3

A.12 Version 0.9.12, August 28, 2015

pbrod (12):

- Updated documentation.
- Updated version in conf.py.
- Updated CHANGES.rst.
- Reimplemented outlier detection and made it more robust.
- Added limits.py with tests.
- Updated main tests folder.
- Moved Richardson and dea3 to extrapolation.py.
- Making a new release in order to upload to pypi.

A.13 Version 0.9.11, August 27, 2015

pbrod (2):

- Fixed sphinx-build and updated docs.
- Fixed issue #9 Backward differentiation method fails with additional parameters.

A.14 Version 0.9.10, August 26, 2015

pbrod (7):

- Fixed sphinx-build and updated docs.
- Added more tests to nd_algopy.
- Dropped support for Python 2.6.

A.15 Version 0.9.4, August 26, 2015

pbrod (7):

- Fixed sphinx-build and updated docs.

A.16 Version 0.9.3, August 23, 2015

Paul Kienzle (1):

- more useful benchmark plots.

pbrod (7):

- Fixed bugs and updated docs.
- Major rewrite of the easy to use interface to Algopy.
- Added possibility to calculate n'th order derivative not just for n=1 in nd_algopy.
- Added tests to the easy to use interface to algopy.

A.17 Version 0.9.2, August 20, 2015

pbrod (3):

- Updated documentation
- Added parenthesis to a call to the print function
- Made the test less strict in order to pass the tests on Travis for python 2.6 and 3.2.

A.18 Version 0.9.1, August 20,2015

Christoph Deil (1):

- Fix Sphinx build

pbrod (47):

- **Total remake of numdifftools with slightly different call syntax.**
  - Can compute derivatives of order up to 10-14 depending on function and method used.
  - Updated documentation and tests accordingly.
  - Fixed a bug in dea3.
  - Added StepsGenerator as an replacement for the adaptive option.
  - Added bicomplex class for testing the complex step second derivative.
  - Added fornberg_weights_all for computing optimal finite difference rules in a stable way.
  - Added higher order complex step derivative methods.

A.19 Version 0.7.7, December 18, 2014

pbrod (35):

- Got travis-ci working in order to run the tests automatically.
- Fixed bugs in Dea class.
- Fixed better error estimate for the Hessian.
- Fixed tests for python 2.6.
- Adding tests as subpackage.
- Restructerd folders of numdifftools.

A.20 Version 0.7.3, December 17, 2014

pbrod (5):

- Small cosmetic fixes.
- pep8 + some refactorings.
- Simplified code by refactoring.

A.21 Version 0.6.0, February 8, 2014

pbrod (20):

- Update and rename README.md to README.rst.
- Simplified call to Derivative: removed step_fix.
- Deleted unused code.
- Simplified and Refactored. Now possible to choose step_num=1.
- Changed default step_nom from max(abs(x0), 0.2) to max(log2(abs(x0)), 0.2).
- pep8ified code and made sure that all tests pass.

A.22 Version 0.5.0, January 10, 2014

pbrod (9):

- Updated the examples in Gradient class and in info.py.
- Added test for vec2mat and docstrings + cosmetic fixes.
- Refactored code into private methods.
- Fixed issue #7: Derivative(fun)(numpy.ones((10,5)) * 2) failed.
- Made print statements compatible with python 3.

A.23 Version 0.4.0, May 5, 2012

pbrod (1)

- Fixed a bug for inf and nan values.

A.24 Version 0.3.5, May 19, 2011

pbrod (1)

- Fixed a bug for inf and nan values.

A.25 Version 0.3.4, Feb 24, 2011

pbrod (11)

- Made automatic choice for the stepsize more robust.
- Added easy to use interface to the algopy and scientificpython modules.

A.26 Version 0.3.1, May 20, 2009

pbrod (4)

- First version of numdifftools published on google.code

APPENDIX

B

CONTRIBUTORS

- Per A. Brodtkorb <per.andreas.brodtkorb (at) gmail.com>
- John D'Errico <woodchips (at) rochester.rr.com>

APPENDIX

C

LICENSE

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```

APPENDIX

D

ACKNOWLEDGMENTS

The numdifftools package was originally a translation of an adaptive numerical differentiation toolbox written in Matlab by John D'Errico [**?**].

Numdifftools has as of version 0.9 been extended with some of the functionality found in the statsmodels.tools.numdiff module written by Josef Perktold [**?**].

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