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# **Numdifftools Documentation**

***Release 0.9.41***

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**Nov 10, 2022**



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This is the documentation of **Numdifftools** version 0.9.41 released Nov 10, 2022.

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

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





## INTRODUCTION

### 1.1 What is numdifftools?

Numdifftools is a suite of tools written in [\\_Python](http://www.python.org/)<sup>5</sup> 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](https://pythonhosted.org/algopy/)<sup>6</sup>. 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.

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<sup>5</sup> <http://www.python.org/>

<sup>6</sup> <https://pythonhosted.org/algopy/>

- *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.

## 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 need 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 latest 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
```

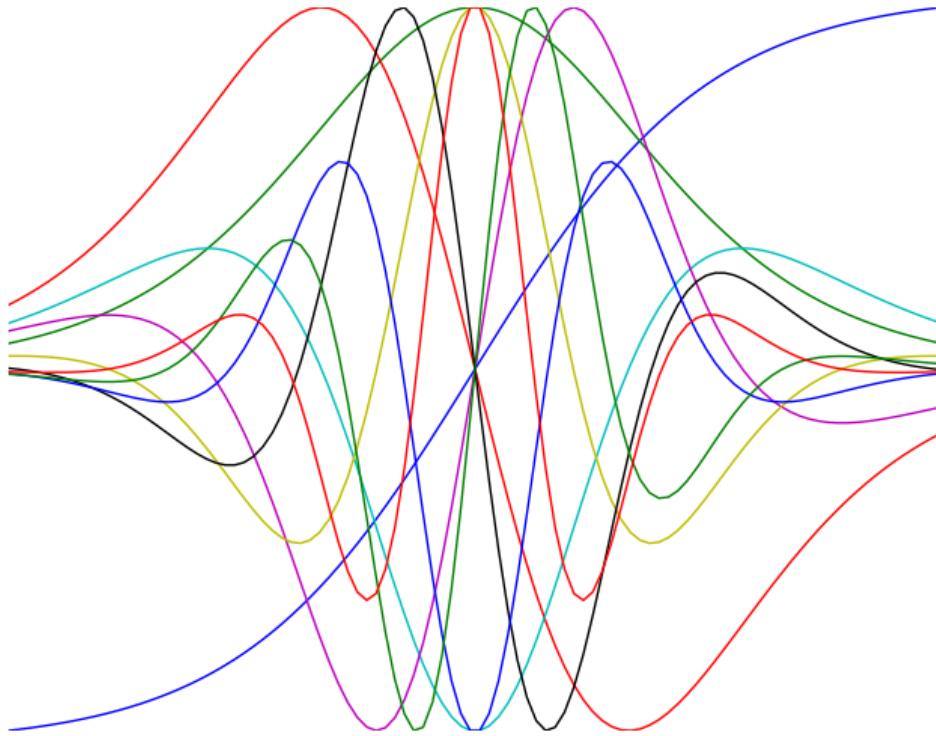
```
>>> dddf = nd.Derivative(sin, n=3)
>>> np.allclose(dddf(0), -1.)
True
```

```
>>> 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()



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### 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.

---

<sup>7</sup> <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,  $x_0 = [1, 1]$ :

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



## 2.3 Conclusion

numdifftools.Derivative is an 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](#)<sup>8</sup> 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](#)<sup>9</sup> 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`.

### 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
```

---

<sup>8</sup> <http://sphinx-doc.org/>

<sup>9</sup> <https://www.gnu.org/software/make/>

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](https://python.org/)<sup>10</sup>, so if you're new to [Python](https://python.org/)<sup>11</sup>, 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](https://wiki.python.org/moin/BeginnersGuide/NonProgrammers)<sup>12</sup>

If you already know a few other languages and want to get up to speed with Python quickly, we recommend [Dive Into Python](https://www.diveinto.org/python3/)<sup>13</sup>. If that's not quite your style, there are many other [books about Python](https://wiki.python.org/moin/PythonBooks)<sup>14</sup>.

---

<sup>10</sup> <https://python.org/>

<sup>11</sup> <https://python.org/>

<sup>12</sup> <https://wiki.python.org/moin/BeginnersGuide/NonProgrammers>

<sup>13</sup> <https://www.diveinto.org/python3/>

<sup>14</sup> <https://wiki.python.org/moin/PythonBooks>



## 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 is 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 something 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 environment 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 environment 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 environment, 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 official 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





## 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 an 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.

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

For small  $\delta$ , the limit approaches  $f'(x)$ . This is a one-sided approximation for the derivative. For a fixed value of  $\delta$ , 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  $x_0$ .

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

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

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

When  $\delta$  is small,  $\delta^2$  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  $\delta$ .<sup>1</sup> The values of  $f''(x_0)$  and  $f'''(x_0)$ , while unknown to us, are fixed constants as  $\delta$  varies.

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

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

### 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<sup>2</sup> 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  $f_{even}(x)$ .

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

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

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  $x_0$ .

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

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  $f(x)$ .

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

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  $\delta$ .

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

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

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

---

<sup>1</sup> 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.

<sup>2</sup> 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  $\delta$  on it, so we would normally ignore it since the lowest order neglected term should dominate the behavior for small  $\delta$ .

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

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  $\delta$  in (4.2) with a complex step  $ih$ :

$$\begin{aligned} f(x_0 + ih) = f(x_0) + ihf'(x_0) - \frac{h^2}{2}f''(x_0) - \frac{ih^3}{6}f^{(3)}(x_0) + \frac{h^4}{24}f^{(4)}(x_0) + \\ \frac{ih^5}{120}f^{(5)}(x_0) - \frac{h^6}{720}f^{(6)}(x_0) - \dots \end{aligned} \quad (4.12)$$

Taking only the imaginary parts of both sides gives

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

Dividing with  $h$  and rearranging yields:

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

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:

$$f'(x_0) = \Im(f(x_0 + ih))/h \quad (4.15)$$

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

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

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

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

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:

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

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 demonstrate 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:

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

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

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

The solution of these equations are simply:

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

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 being 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  $\delta$  at a fixed  $x_0$ . Thus, choose a single  $\delta$ , 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  $\delta \rightarrow 0$ , 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  $\delta$  is small enough that the linear term dominates so we can ignore the quadratic term, therefore the error is purely linear.

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

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

$$f'_0 = 2f'_{\delta/2} - f'_\delta \quad (4.23)$$

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  $\delta$  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  $\delta$  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  $\delta$  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  $\delta$ . Again, assume the step size is cut in half again. The three term Richardson extrapolant is given by:

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

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<sup>3</sup>. 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  $f_{\text{odd}}(\delta)/\delta$  by rearranging (4.19):

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

This equation has the form

$$\phi(\delta) = L + a_0\delta^2 + a_1\delta^4 + a_2\delta^6 + \dots \quad (4.26)$$

<sup>3</sup> 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  $f_{\text{odd}}(\delta)/\delta$ .

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:

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

The solution of these equations are simply:

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

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  $\delta$ . 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  $\delta$ , 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)
```

(continues on next page)

(continued from previous page)

```
>>> 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.





## REFERENCE

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

### 5.1 Numdifftools summary

#### 5.1.1 numdifftools.core module

<i>Derivative</i> (page 73)(fun[, step, method, order, n])	Calculate n-th derivative with finite difference approximation
<i>Gradient</i> (page 75)(fun[, step, method, order, n])	Calculate Gradient with finite difference approximation
<i>Jacobian</i> (page 82)(fun[, step, method, order, n])	Calculate Jacobian with finite difference approximation
<i>Hessdiag</i> (page 77)(f[, step, method, order])	Calculate Hessian diagonal with finite difference approximation
<i>Hessian</i> (page 79)(f[, step, method, order])	Calculate Hessian with finite difference approximation
<i>directionaldiff</i> (page 87)(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, \*\*kwargs)

**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 75)

[Hessian](#) (page 79)

### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

<code>__init__(fun, step=None, method='central', order=2, n=1, **options)</code>	Initialize self. See help(type(self)) for accurate signature.
--	---

## Methods

<code>__init__</code> (page 29)(fun[, step, method, order, n])	Initialize self.
<code>set_richardson_rule</code> (page 75)(step_ratio[, num_terms])	Set Richardson extrapolation options

## Attributes

<code>method</code> (page 75)	Defines the method used in the finite difference approximation.
<code>method_order</code> (page 75)	Defines the leading order of the error term in the Richardson extrapolation method.
<code>n</code> (page 75)	Order of the derivative.
<code>order</code> (page 75)	Defines the order of the error term in the Taylor approximation used.
<code>step</code> (page 75)	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, **kws)`

**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 73), [Hessian](#) (page 79), [Jacobian](#) (page 82)

#### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $n \times m$  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  $\sin(x-y) + y \cdot \exp(x)$

```
>>> 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

`__init__(fun, step=None, method='central', order=2, n=1, **options)`  
 Initialize self. See help(type(self)) for accurate signature.

## Methods

<code>__init__</code> (page 31)( <code>fun</code> [, <code>step</code> , <code>method</code> , <code>order</code> , <code>n</code> ])	Initialize self.
<code>set_richardson_rule</code> (page 77)( <code>step_ratio</code> [, <code>num_terms</code> ])	Set Richardson extrapolation options

## Attributes

<code>method</code> (page 77)	Defines the method used in the finite difference approximation.
<code>method_order</code> (page 77)	Defines the leading order of the error term in the Richardson extrapolation method.
<code>n</code> (page 77)	Order of the derivative.
<code>order</code> (page 77)	Defines the order of the error term in the Taylor approximation used.
<code>step</code> (page 77)	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, **kws)`

**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 73), [Hessian](#) (page 79), [Gradient](#) (page 75)

## 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $\text{fun}(x)$  does not support complex numbers or involves non-analytic functions such as e.g.:  $\text{abs}$ ,  $\text{max}$ ,  $\text{min}$ . 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  $\text{fun}$  returns a 1d array, it returns a Jacobian. If a 2d array is returned by  $\text{fun}$  (e.g., with a value for each observation), it returns a 3d array with the Jacobian of each observation with shape  $xk \times \text{nobs} \times xk$ . 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

`__init__(fun, step=None, method='central', order=2, n=1, **options)`  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

<code>__init__</code> (page 34)(fun[, step, method, order, n])	Initialize self.
<code>set_richardson_rule</code> (page 84)(step_ratio[, num_terms])	Set Richardson extrapolation options

---

## Attributes

---

<code>method</code> (page 84)	Defines the method used in the finite difference approximation.
<code>method_order</code> (page 84)	Defines the leading order of the error term in the Richardson extrapolation method.
<code>n</code> (page 84)	Order of the derivative.
<code>order</code> (page 84)	Defines the order of the error term in the Taylor approximation used.
<code>step</code> (page 84)	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, \*\*kwargs)

**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

**hessdiag** [array] hessian diagonal

See also:

[Derivative](#) (page 73), [Hessian](#) (page 79), [Jacobian](#) (page 82), [Gradient](#) (page 75)

#### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $\text{fun}(x)$  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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

`__init__(f, step=None, method='central', order=2, **options)`  
 Initialize self. See help(type(self)) for accurate signature.

## Methods

---

<code>__init__</code> (page 36)(f[, step, method, order])	Initialize self.
<code>set_richardson_rule</code> (page 79)(step_ratio[, num_terms])	Set Richardson extrapolation options

---

## Attributes

---

<code>method</code> (page 79)	Defines the method used in the finite difference approximation.
<code>method_order</code> (page 79)	Defines the leading order of the error term in the Richardson extrapolation method.
<code>n</code> (page 79)	Order of the derivative.
<code>order</code> (page 79)	Defines the order of the error term in the Taylor approximation used.
<code>step</code> (page 79)	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, \*\*kwargs)

**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 73), [Hessian](#) (page 79)

### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $\text{fun}(x)$  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):

$$((f(x + d_j e_j + d_k e_k) + f(x) - f(x + d_j e_j) - f(x + d_k e_k)))/(d_j d_k) \quad (5.1)$$

$$((f(x + d_j e_j + d_k e_k) - f(x + d_j e_j - d_k e_k)) - (f(x - d_j e_j + d_k e_k) - f(x - d_j e_j - d_k e_k)))/(4d_j d_k) \quad (5.2)$$

$$\text{imag}(f(x + id_j e_j + d_k e_k) - f(x + id_j e_j - d_k e_k))/(2d_j d_k) \quad (5.3)$$

where  $e_j$  is a vector with element  $j$  is one and the rest are zero and  $d_j$  is a scalar spacing  $\text{steps}_j$ .

### 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

`__init__(f, step=None, method='central', order=None, **options)`  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

<code>__init__</code> (page 38)(f[, step, method, order])	Initialize self.
<code>set_richardson_rule</code> (page 82)(step_ratio[, num_terms])	Set Richardson extrapolation options

---

## Attributes

---

<code>method</code> (page 81)	Defines the method used in the finite difference approximation.
<code>method_order</code> (page 81)	Defines the leading order of the error term in the Richardson extrapolation method.
<code>n</code> (page 81)	Order of the derivative.
<code>order</code> (page 81)	Defines the order of the error term in the Taylor approximation used.
<code>step</code> (page 82)	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 *n*×*m* 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 73)

[Gradient](#) (page 75)

#### 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

<i>BasicMaxStepGenerator</i> (page 121)(base_step, step_ratio, ...)	Generates a sequence of steps of decreasing magnitude
<i>BasicMinStepGenerator</i> (page 122)(base_step, step_ratio, ...)	Generates a sequence of steps of decreasing magnitude
<i>MinStepGenerator</i> (page 123)([base_step, step_ratio, ...])	Generates a sequence of steps
<i>MaxStepGenerator</i> (page 122)([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**  $\text{steps} = \text{base\_step} * \text{step\_ratio} ** (-i + \text{offset})$

for  $i=0, 1, \dots, \text{num\_steps}-1$ .

#### 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*)

Initialize self. See help(type(self)) for accurate signature.

#### Methods

---

**\_\_init\_\_** (page 40)(*base\_step, step\_ratio, num\_steps[, ...]*) Initialize self.

---

### 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**  $\text{steps} = \text{base\_step} * \text{step\_ratio} ** (i + \text{offset}), i=\text{num\_steps}-1, \dots, 1, 0$ .

#### 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)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

**\_\_init\_\_** (page 41)(*base\_step*, *step\_ratio*, Initialize self.  
*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**  $\text{steps} = \text{step\_nom} * \text{base\_step} * \text{step\_ratio} ** (i + \text{offset})$

for  $i = \text{num\_steps}-1, \dots, 1, 0$ .

#### Parameters

**base\_step** [float, array-like, optional] Defines the minimum step, if None, the value is set to  $\text{EPS} ** (1/\text{scale})$

**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  $\text{min\_num\_steps} + \text{num\_extrap}$ ] defines number of steps generated. It should be larger than  $\text{min\_num\_steps} = (n + \text{order} - 1) / \text{fact}$  where fact is 1, 2 or 4 depending on differentiation method used.

**step\_nom** [default  $\text{maximum}(\log(\exp(1)+|x|), 1)$ ] Nominal step where  $x$  is supplied at run-time 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)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<code>__init__</code> (page 41)([base_step, step_ratio, num_steps, ...])	Initialize self.
<code>step_generator_function</code> (page 123)(x[, method, n, order])	Step generator function

## Attributes

<code>base_step</code> (page 123)	Base step defines the minimum or maximum step when offset==0.
<code>min_num_steps</code> (page 123)	Minimum number of steps required given the differentiation method and order.
<code>num_steps</code> (page 123)	Defines number of steps generated
<code>scale</code> (page 123)	Scale used in base step.
<code>step_nom</code> (page 123)	Nominal step
<code>step_ratio</code> (page 123)	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  $\text{EPS}^{**}(1/\text{scale})$

**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 run-time 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*)  
Initialize self. See help(type(self)) for accurate signature.



## Methods

<code>__init__</code> (page 42)([base_step, step_ratio, num_steps, ...])	Initialize self.
<code>step_generator_function</code> (x[, method, n, order])	Step generator function

## Attributes

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

## 5.1.3 numdifftools.extrapolation module

<code>convolve</code> (page 90)(sequence, rule, **kwds)	Wrapper around <code>scipy.ndimage.convolve1d</code> that allows complex input.
<code>Dea</code> (page 88)([limexp])	Extrapolate a slowly convergent sequence using repeated Shanks transformations.
<code>dea3</code> (page 90)(v_0, v_1, v_2[, symmetric])	Extrapolate a slowly convergent sequence using Shanks transformations.
<code>Richardson</code> (page 89)([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*)

Initialize self. See help(type(self)) for accurate signature.

## Methods

---

`__init__` (page 44)(*limexp*)

Initialize self.

---

## Attributes

---

*limexp* (page 89)

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 88)

## 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 =  $k_1 - k_0 = k_2 - k_1 = \dots = k_{i+1} - k_i$
- 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

$$L = f(h) + a_0 * h^{k_0} + a_1 * h^{k_1} + a_2 * h^{k_2} + \dots$$

where the  $a_i$  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  $L = f(h) + O(h^{k_0})$  ( $f(h) \rightarrow L$  as  $h \rightarrow 0$ , but  $f(0) \neq L$ ) and  $k_i = \text{order} + \text{step} * i$ .

## 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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<code>__init__</code> (page 46)([ <i>step_ratio, step, order, num_terms</i> ])	Initialize self.
<code>extrapolate</code> (page 90)( <i>sequence, steps</i> )	Extrapolate sequence
<code>rule</code> (page 90)([ <i>sequence_length</i> ])	Returns extrapolation rule.

## 5.1.4 numdifftools.limits module

<code>CStepGenerator</code> (page 102)([ <i>base_step, step_ratio, ...</i> ])	Generates a sequence of steps
<code>Limit</code> (page 103)( <i>fun[, step, method, order, full_output]</i> )	Compute limit of a function at a given point
<code>Residue</code> (page 105)( <i>f[, step, method, order, ...]</i> )	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**  $\text{steps} = \text{base\_step} * \text{step\_nom} * (\exp(1j * d\theta) * \text{step\_ratio}) ** (i + \text{offset})$

for  $i = 0, 1, \dots, \text{num\_steps}-1$

#### Parameters

**base\_step** [float, array-like, default None] Defines the minimum step, if None, the value is set to  $\text{EPS} ** (1/\text{scale})$

**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  $2 * \text{int}(\text{round}(16.0/\log(\text{abs}(\text{step\_ratio})))) + 1$

**step\_nom** [default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at run-time 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*)

Initialize self. See help(type(self)) for accurate signature.

## Methods

---

**\_\_init\_\_** (page 47)(*[base\_step, step\_ratio, Initialize self. num\_steps, ...]*)

---

**step\_generator\_function**(*x[, method, n, Step generator function order]*)

---

## Attributes

<code>base_step</code>	Base step defines the minimum or maximum step when offset==0.
<code>dtheta</code> (page 103)	Angular steps in radians used for the exponential spiral path.
<code>min_num_steps</code>	Minimum number of steps required given the differentiation method and order.
<code>num_steps</code> (page 103)	The number of steps generated
<code>scale</code>	Scale used in base step.
<code>step_nom</code>	Nominal step
<code>step_ratio</code> (page 103)	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, **kws)` to compute the limit for  $z \rightarrow z_0$ . 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  $z \rightarrow z_0$

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

**error\_estimate:** ndarray 95 % uncertainty estimate around the limit, such that  $\text{abs}(\text{limit\_fz} - \lim_{z \rightarrow z_0} f(z)) < \text{error\_estimate}$

**final\_step:** ndarray final step used in approximation

## Notes

*Limit* computes the limit of a given function at a specified point,  $z_0$ . 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  $z_0$ .  $z_0$  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  $z_0$  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  $z_0$  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  $z*\text{fun}(z)$  as  $z \rightarrow 0$ . 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  $z**2*\text{fun}(z)$  as  $z \rightarrow 0$ .

```
>>> 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.expml(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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<code>__init__</code> (page 49)( <i>fun</i> [, <i>step</i> , <i>method</i> , <i>order</i> , <i>full_output</i> ])	Initialize self.
<code>limit</code> (page 104)( <i>x</i> , <i>*args</i> , <i>**kwds</i> )	Return $\lim f(z)$ as $z \rightarrow x$

## Attributes

<code>step</code>	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  $z=z_0$ . 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  $z_0$ .

**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  $f(z)*(z-z_0)^{pole\_order}$  as  $z \rightarrow z_0$  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  $abs(res\_fz - \lim_{z \rightarrow z_0} f(z)*(z-z_0)^{pole\_order}) < error\_estimate$  Large uncertainties here suggest that the wrong order pole was specified for  $f(z_0)$ .

**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*)  
Initialize self. See help(type(self)) for accurate signature.

#### Methods

<code>__init__</code> (page 50)( <i>f</i> , <i>step</i> , <i>method</i> , <i>order</i> , ... )	Initialize self.
<code>limit</code> ( <i>x</i> , <i>*args</i> , <i>**kwargs</i> )	Return $\lim_{z \rightarrow x} f(z)$



## Attributes

<code>step</code>	The step spacing(s) used in the approximation
-------------------	---

## 5.1.5 numdifftools.multicomplex module

<code>Bicomplex</code> (page 106)( <i>z1</i> , <i>z2</i> )	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'>)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<code>__init__</code> (page 51)( <i>z1</i> , <i>z2</i> [, <i>dtype</i> ])	Initialize self.
<code>arccos</code> (page 106)()	
<code>arccosh</code> (page 106)()	
<code>arcsin</code> (page 106)()	
<code>arcsinh</code> (page 106)()	
<code>arctan</code> (page 106)()	
<code>arctanh</code> (page 106)()	
<code>arg_c</code> (page 106)()	
<code>arg_clp</code> (page 106)()	
<code>asarray</code> (page 106)(other)	
<code>conjugate</code> (page 106)()	
<code>cos</code> (page 106)()	
<code>cosh</code> (page 106)()	
<code>cot</code> (page 106)()	
<code>coth</code> (page 106)()	
<code>csc</code> (page 106)()	
<code>csch</code> (page 106)()	
<code>dot</code> (page 106)(other)	
<code>exp</code> (page 106)()	
<code>exp2</code> (page 106)()	
<code>expm1</code> (page 106)()	
<code>flat</code> (page 107)(index)	
<code>log</code> (page 107)()	
<code>log10</code> (page 107)()	
<code>log1p</code> (page 107)()	
<code>log2</code> (page 107)()	
<code>logaddexp</code> (page 107)(other)	
<code>logaddexp2</code> (page 107)(other)	
<code>mat2bicomplex</code> (page 107)(arr)	
<code>mod_c</code> (page 107)()	Complex modulus
<code>norm</code> (page 107)()	
<code>sec</code> (page 107)()	
<code>sech</code> (page 107)()	

continues on next page

Table 5.36 – continued from previous page

<a href="#"><i>sin</i></a> (page 107)()
<a href="#"><i>sinh</i></a> (page 107)()
<a href="#"><i>sqrt</i></a> (page 107)()
<a href="#"><i>tan</i></a> (page 107)()
<a href="#"><i>tanh</i></a> (page 107)()

### Attributes

<a href="#"><i>imag</i></a> (page 107)
<a href="#"><i>imag1</i></a> (page 107)
<a href="#"><i>imag12</i></a> (page 107)
<a href="#"><i>imag2</i></a> (page 107)
<a href="#"><i>real</i></a> (page 107)
<a href="#"><i>shape</i></a> (page 107)
<a href="#"><i>size</i></a> (page 107)
<a href="#"><i>z1</i></a> (page 107)
<a href="#"><i>z2</i></a> (page 107)

## 5.1.6 numdifftools.nd\_algopy module

<a href="#"><i>Derivative</i></a> (page 108)(fun[, n, method, full_output])	Calculate n-th derivative with Algorithmic Differentiation method
<a href="#"><i>Gradient</i></a> (page 109)(fun[, n, method, full_output])	Calculate Gradient with Algorithmic Differentiation method
<a href="#"><i>Jacobian</i></a> (page 113)(fun[, n, method, full_output])	Calculate Jacobian with Algorithmic Differentiation method
<a href="#"><i>Hessdiag</i></a> (page 111)(f[, method, full_output])	Calculate Hessian diagonal with Algorithmic Differentiation method
<a href="#"><i>Hessian</i></a> (page 112)(f[, method, full_output])	Calculate Hessian with Algorithmic Differentiation method
<a href="#"><i>directionaldiff</i></a> (page 115)(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, \*\*kws)

**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 109)

[\*Hessdiag\*](#) (page 111)

[Hessian](#) (page 112)

[Jacobian](#) (page 113)

## 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](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

<b><code>__call__</code>:</b> callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
---	--

**`__init__`** (*fun*, *n=1*, *method='forward'*, *full\_output=False*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

<code>__init__</code>	(page 53)	( <code>fun</code> [, <code>n</code> , <code>method</code> , <code>Initialize self.</code> <code>full_output</code> ])
<code>computational_graph</code>	( <code>x</code> , <code>*args</code> , <code>**kwargs</code> )	

---

## Attributes

---

<code>fun</code>
------------------

---

### 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, **kwargs)`

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

#### Returns

**grad: array** gradient

See also:

[\*Derivative\*](#) (page 108)

[\*Jacobian\*](#) (page 113)

[\*Hessdiag\*](#) (page 111)

[\*Hessian\*](#) (page 112)

## 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](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

<b><code>__call__</code>: callable with the following parameters:</b>	<code>x</code> : array_like value at which function derivative is evaluated <code>args</code> : tuple Arguments for function <i>fun</i> . <code>kwds</code> : dict Keyword arguments for function <i>fun</i> .
---	--

**`__init__`** (*fun, n=1, method='forward', full\_output=False*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

**`__init__`** (page 55)(*fun[, n, method, Initialize self. 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, **kws)`

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

#### Returns

**jacob: array** Jacobian

See also:

[Derivative](#) (page 108)

[Gradient](#) (page 109)

[Hessdiag](#) (page 111)

[Hessian](#) (page 112)

#### 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwargs: dict Keyword arguments for function <i>fun</i> .
--	--

**`__init__`** (*fun*, *n*=1, *method*='forward', *full\_output*=False)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

<code>__init__</code>	(page 57)	( <code>fun</code> [, <code>n</code> , <code>method</code> , <code>Initialize self.</code> <code>full_output</code> ])
<code>computational_graph</code>	( <code>x</code> , <code>*args</code> , <code>**kwargs</code> )	

---

## Attributes

---

<code>fun</code>
------------------

---

### 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, **kwargs)`

**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 108)

[Gradient](#) (page 109)

[Jacobian](#) (page 113)

[Hessian](#) (page 112)

## 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**`__init__`** (*f*, *method*='forward', *full\_output*=False)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<a href="#"><code>__init__</code></a> (page 59)( <i>f</i> , <i>method</i> , <i>full_output</i> )	Initialize self.
<code>computational_graph</code> ( <i>x</i> , *args, **kwds)	

## Attributes

<code>fun</code>
------------------

### 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, **kws)`

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

#### Returns

**hess** [ndarray] array of partial second derivatives, Hessian

See also:

[\*Derivative\*](#) (page 108)

[\*Gradient\*](#) (page 109)

[\*Jacobian\*](#) (page 113)

[\*Hessdiag\*](#) (page 111)

#### 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**`__init__`** (*f*, *method*='forward', *full\_output*=False)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

<b><code>__init__</code></b> (page 61)( <i>f</i> , <i>method</i> , <i>full_output</i> )	Initialize self.
<b><code>computational_graph</code></b> ( <i>x</i> , *args, **kwds)	

## Attributes

<b><code>fun</code></b>
-------------------------

### 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 108)

[Gradient](#) (page 109)

## 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

<a href="#">Gradient</a> (page 116)(fun[, step, method, order, bounds, ...])	Calculate Gradient with finite difference approximation
<a href="#">Jacobian</a> (page 117)(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, \*\*kws)

**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 117)

## 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])
```

(continues on next page)

(continued from previous page)

```
>>> 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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

**\_\_init\_\_** (page 63)(*fun[, step, method, order, bounds, ...]*) Initialize self.

---

### 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, \*\*kws*)

**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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

`__init__` (page 64)(*fun*[, *step*, *method*, *order*, *bounds*, ...]) Initialize self.

---

## 5.1.8 numdifftools.nd\_statsmodels module

<code>Hessian</code> (page 118)( <i>fun</i> [, <i>step</i> , <i>method</i> , <i>order</i> ])	Calculate Hessian with finite difference approximation
<code>Jacobian</code> (page 119)( <i>fun</i> [, <i>step</i> , <i>method</i> , <i>order</i> ])	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, **kws)`

**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 119), `Gradient` (page 118)

## 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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

**\_\_init\_\_** (page 65)(*fun[, step, method, order]*) Initialize self.

---

## Attributes

---

**method**

---

**n** (page 119)

---

**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, \*\*kws)*

**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*)  
Initialize self. See help(type(self)) for accurate signature.

## Methods

---

`__init__` (page 66)(*fun*[, *step*, *method*, *order*]) Initialize self.

---

## 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`<sup>15</sup>

Hamiltonian

#### Parameters

**n** [scalar] number of ions in the chain

---

<sup>15</sup> <https://docs.python.org/3.8/library/functions.html#object>



**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  $V_x$  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`<sup>16</sup>

**setup\_method** ()

**test\_dea3\_on\_trapz\_sin** ()

**test\_dea\_on\_trapz\_sin** ()

**test\_epsal** ()

**test\_richardson** ()

**class TestRichardson**

Bases: `object`<sup>17</sup>

**setup\_method** ()

**test\_order\_step\_combinations** ()

### 5.2.1.3 numdifftools.tests.test\_fornberg module

**class ExampleFunctions**

Bases: `object`<sup>18</sup>

**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)

---

<sup>16</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>17</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>18</sup> <https://docs.python.org/3.8/library/functions.html#object>

```
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 () → None19
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: object20
    static test_default_base_step ()
    static test_default_generator ()
    static test_fixed_base_step ()

class TestLimit
    Bases: object21
    test_derivative_of_cos ()
    test_difficult_limit ()
    test_residue_1_div_1_minus_exp_x ()
    test_sinx_div_x ()

class TestResidue
    Bases: object22
    test_residue_1_div_1_minus_exp_x ()
    test_residue_1_div_sin_x2 ()
```

---

<sup>20</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>21</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>22</sup> <https://docs.python.org/3.8/library/functions.html#object>

### 5.2.1.5 numdifftools.tests.test\_multicomplex module

Created on 22. apr. 2015

@author: pab

```
class TestBicomplex
    Bases: object23

    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()
    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()
```

---

<sup>23</sup> <https://docs.python.org/3.8/library/functions.html#object>

```
    static test_sub()
    static test_subsref()
class TestDerivative
    Bases: object24
    static test_all_first_derivatives()
    static test_all_second_derivatives()
```

#### 5.2.1.6 numdifftools.tests.test\_nd\_algopy module

```
class TestDerivative
    Bases: object25
    static test_derivative_cube()
        Test for Issue 7
    static test_derivative_exp() → None26
    static test_derivative_on_log() → None27
    static test_derivative_on_sinh() → None28
    static test_derivative_sin()
    static test_directional_diff()
    static test_fun_with_additional_parameters()
        Test for issue #9
    static test_high_order_derivative_cos()

class TestGradient
    Bases: object29
    static test_on_scalar_function()

class TestHessdiag
    Bases: object30
    static test_forward()
    static test_reverse()

class TestHessian
    Bases: object31
    static test_hessian_cos_x_y_at_0_0()
    test_run_hamiltonian()

class TestJacobian
    Bases: object32
    static test_issue_25()
    static test_on_matrix_valued_function()
    static test_on_scalar_function()
    static test_on_vector_valued_function()
    static test_scalar_to_vector() → None33
```

---

<sup>24</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>25</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>29</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>30</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>31</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>32</sup> <https://docs.python.org/3.8/library/functions.html#object>

### 5.2.1.7 numdifftools.tests.test\_nd\_scipy module

```
class TestGradient
    Bases: object34

    static test_on_scalar_function ()

class TestJacobian
    Bases: object35

    test_issue_25 ()

    test_on_matrix_valued_function ()

    static test_on_scalar_function ()

    test_on_vector_valued_function ()

    static test_scalar_to_vector () → None36
```

### 5.2.1.8 numdifftools.tests.test\_numdifftools module

Test functions for numdifftools module

```
class TestDerivative
    Bases: object37

    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 () → None38

    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: object39

    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.
```

---

<sup>34</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>35</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>37</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>39</sup> <https://docs.python.org/3.8/library/functions.html#object>

```
    static test_issue_39 ()
        Test that checks float/Bicomplex works
class TestHessdiag
    Bases: object40
    test_complex ()
    test_default_step ()
    test_fixed_step () → None41
class TestHessian
    Bases: object42
    test_complex_hessian_issue_35 ()
    static test_hessian_cos_x_y_at_0_0 ()
    test_run_hamiltonian ()
class TestJacobian
    Bases: object43
    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 () → None44
class TestRichardson
    Bases: object45
    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 ()
```

---

<sup>40</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>42</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>43</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>45</sup> <https://docs.python.org/3.8/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: numdifftools.limits.\_Limit

Calculate n-th derivative with finite difference approximation

#### Parameters

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

**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 75)

[Hessian](#) (page 79)

## 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $\text{fun}(x)$  does not support complex numbers or involves non-analytic functions such as e.g.:  $\text{abs}$ ,  $\text{max}$ ,  $\text{min}$ . 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

**class info** (*f\_value, error\_estimate, final\_step, index*)

Bases: `tuple`<sup>46</sup>

**count** (*value, /*)

Return number of occurrences of value.

**error\_estimate**

Alias for field number 1

**f\_value**

Alias for field number 0

**final\_step**

Alias for field number 2

**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 extrapolation options

**property step**

The step spacing(s) used in the approximation

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

Bases: `numdifftools.core.Jacobian` (page 82)

Calculate Gradient with finite difference approximation

### Parameters

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

**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.

---

<sup>46</sup> <https://docs.python.org/3.8/library/stdtypes.html#tuple>

**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 73), [Hessian](#) (page 79), [Jacobian](#) (page 82)

### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $\text{fun}(x)$  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  $x_0$  is an  $n \times m$  array, then  $\text{fun}$  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
>>> grad_rosen = nd.Gradient(rosen)
>>> df_dx, df_dy = grad_rosen([x, y])
>>> np.allclose([df_dx, df_dy], [0, 0])
True

```

## Methods

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

**class info** (*f\_value, error\_estimate, final\_step, index*)

Bases: `tuple`<sup>47</sup>

**count** (*value, /*)

Return number of occurrences of value.

**error\_estimate**

Alias for field number 1

**f\_value**

Alias for field number 0

**final\_step**

Alias for field number 2

**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 extrapolation options

**property step**

The step spacing(s) used in the approximation

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

Bases: `numdifftools.core.Derivative` (page 73)

Calculate Hessian diagonal with finite difference approximation

---

<sup>47</sup> <https://docs.python.org/3.8/library/stdtypes.html#tuple>

### Parameters

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

**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

**hessdiag** [array] hessian diagonal

See also:

[Derivative](#) (page 73), [Hessian](#) (page 79), [Jacobian](#) (page 82), [Gradient](#) (page 75)

### 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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

**class info** (*f\_value, error\_estimate, final\_step, index*)

Bases: `tuple`<sup>48</sup>

**count** (*value, /*)

Return number of occurrences of value.

**error\_estimate**

Alias for field number 1

**f\_value**

Alias for field number 0

**final\_step**

Alias for field number 2

**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 extrapolation options

**property step**

The step spacing(s) used in the approximation

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

Bases: `numdifftools.core.Hessdiag` (page 77)

Calculate Hessian with finite difference approximation

**Parameters**

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

---

<sup>48</sup> <https://docs.python.org/3.8/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

**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 73), [Hessian](#) (page 79)

### 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  $O(\text{steps}^2)$  for  $n=1$  and  $O(\text{steps}^4)$  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  $\text{fun}(x)$  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):

$$((f(x + d_j e_j + d_k e_k) + f(x) - f(x + d_j e_j) - f(x + d_k e_k)))/(d_j d_k) \quad (5.4)$$

$$((f(x + d_j e_j + d_k e_k) - f(x + d_j e_j - d_k e_k)) - (f(x - d_j e_j + d_k e_k) - f(x - d_j e_j - d_k e_k)))/(4d_j d_k) \quad (5.5)$$

$$\text{imag}(f(x + id_j e_j + d_k e_k) - f(x + id_j e_j - d_k e_k))/(2d_j d_k) \quad (5.6)$$

where  $e_j$  is a vector with element  $j$  is one and the rest are zero and  $d_j$  is a scalar spacing  $\text{steps}_j$ .

### 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

**class info** (*f\_value*, *error\_estimate*, *final\_step*, *index*)

Bases: `tuple`<sup>49</sup>

**count** (*value*, /)

Return number of occurrences of value.

**error\_estimate**

Alias for field number 1

**f\_value**

Alias for field number 0

**final\_step**

Alias for field number 2

**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.

---

<sup>49</sup> <https://docs.python.org/3.8/library/stdtypes.html#tuple>

**property order**

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

**set\_richardson\_rule** (*step\_ratio*, *num\_terms*=2)

Set Richardson extrapolation options

**property step**

The step spacing(s) used in the approximation

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

Bases: [numdifftools.core.Derivative](#) (page 73)

Calculate Jacobian with finite difference approximation

**Parameters**

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

**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 73), [Hessian](#) (page 79), [Gradient](#) (page 75)

**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  $O(\text{steps}^{**2})$  for  $n=1$  and  $O(\text{steps}^{**4})$  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  $x_k \times \text{nobs} \times x_k$ . 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

---

<code>__call__(x, *args, **kwargs)</code>	Call self as a function.
---	--------------------------

---

**class info** (*f\_value, error\_estimate, final\_step, index*)

Bases: `tuple`<sup>50</sup>

**count** (*value, /*)

Return number of occurrences of value.

**error\_estimate**

Alias for field number 1

**f\_value**

Alias for field number 0

**final\_step**

Alias for field number 2

**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 extrapolation 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: `numdifftools.step_generators.MinStepGenerator` (page 123)

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 run-time through the `__call__` method.

---

<sup>50</sup> <https://docs.python.org/3.8/library/stdtypes.html#tuple>

**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`<sup>51</sup>

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 run-time 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.

<sup>51</sup> <https://docs.python.org/3.8/library/functions.html#object>

**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`<sup>52</sup>

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  
=  $k_1 - k_0 = k_2 - k_1 = \dots = k_{i+1} - k_i$

**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

$$L = f(h) + a_0 * h^{k_0} + a_1 * h^{k_1} + a_2 * h^{k_2} + \dots$$

where the  $a_i$  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  $L = f(h) + O(h^{k_0})$  ( $f(h) \rightarrow L$  as  $h \rightarrow 0$ , but  $f(0) \neq L$ ) and  $k_i = \text{order} + \text{step} * i$ .

## 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)
```

(continues on next page)

---

<sup>52</sup> <https://docs.python.org/3.8/library/functions.html#object>

(continued from previous page)

```
>>> 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:

**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 *n*×*m* 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 73)[Gradient](#) (page 75)**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`<sup>53</sup>

Extrapolate a slowly convergent sequence using repeated Shanks transformations.

---

<sup>53</sup> <https://docs.python.org/3.8/library/functions.html#object>

## 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`<sup>54</sup>

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`<sup>55</sup>

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.,  $\text{step} = k_1 - k_0 = k_2 - k_1 = \dots = k_{i+1} - k_i$

**order: scalar integer** Leading order of truncation error.

<sup>54</sup> <https://docs.python.org/3.8/library/functions.html#object>

<sup>55</sup> <https://docs.python.org/3.8/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

$$L = f(h) + a_0 * h^{k_0} + a_1 * h^{k_1} + a_2 * h^{k_2} + \dots$$

where the  $a_i$  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  $L = f(h) + O(h^{k_0})$  ( $f(h) \rightarrow L$  as  $h \rightarrow 0$ , but  $f(0) \neq L$ ) and  $k_i = \text{order} + \text{step} * i$ .

## 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.

**convolve** (*sequence, rule, \*\*kws*)

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 88)



## 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
16             0.99919668      0.99999988      0.00000012
```

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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 absolute 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      0.9999274      0.00000726
32            0.99979919      0.9999955      0.00000045
64            0.99994980      0.9999997      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`<sup>56</sup>

Class defining difference functions

### Notes

The d

**class** **HessdiagDifferenceFunctions**Bases: `object`<sup>57</sup>

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`<sup>58</sup>

Class defining Hessian difference functions

---

<sup>56</sup> <https://docs.python.org/3.8/library/functions.html#object><sup>57</sup> <https://docs.python.org/3.8/library/functions.html#object><sup>58</sup> <https://docs.python.org/3.8/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`<sup>59</sup>

Class defining Jacobian difference functions

#### **static increments** (*n*, *h*)

Returns Jacobian steps

### **class** LogHessdiagRule (*n=1*, *method='central'*, *order=2*)

Bases: `numdifftools.finite_difference.LogRule` (page 95)

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)
>>> 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)
```

<sup>59</sup> <https://docs.python.org/3.8/library/functions.html#object>

```
>>> np.allclose(fder, [[-1., -1.], [-1., -1.]])
True
```

**property** `n`

**class** `LogHessianRule` (*n=1, method='central', order=2*)

Bases: `numdifftools.finite_difference.LogRule` (page 95)

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: `numdifftools.finite_difference.LogRule` (page 95)

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`<sup>60</sup>

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])
```

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<sup>60</sup> <https://docs.python.org/3.8/library/functions.html#object>

(continued from previous page)

```
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`<sup>61</sup>

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 coefficients 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 coefficients is returned (default). If *full\_output* is True, then (*coefs*, *status*) is returned

#### Returns

- coefs** [ndarray] array of taylor coefficients
- 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.

<sup>61</sup> <https://docs.python.org/3.8/library/functions.html#object>

## 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  $z_0 = 0$ :

```
>>> 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*, *\*\*kws*)

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.

**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  $z_0 = 0$ :

```
>>> 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** ( $f(x, x, n=1, m=2)$ )

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  $\text{len}(x) > n$ .

**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:  $0 < n < \text{len}(x)$  and  $2*mm+2 \leq \text{len}(x)$

See also:

[\*fd\\_weights\*](#) (page 100)

## 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 100)

## 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* ( $0 \leq j \leq n$ )

See also:

[\*fd\\_weights\*](#) (page 100)

## Notes

The  $x$  values can be arbitrarily spaced but must be distinct and  $\text{len}(x) > n$ .

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](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*, *\*\*kws*)

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 coefficients 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  $\text{max\_iter} // 2$ ] 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 coefficients is returned (default). If *full\_output* is True, then (coefs, status) is returned

### Returns

**coefs** [ndarray] array of taylor coefficients

**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  $z_0 = 0$ :

```
>>> 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](mailto: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: *numdifftools.step\_generators.MinStepGenerator* (page 123)

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  $\text{EPS}^{**}(1/\text{scale})$

**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  $2 * \text{int}(\text{round}(16.0/\log(\text{abs}(\text{step\_ratio})))) + 1$

**step\_nom** [default maximum(log(exp(1)+|x|), 1)] Nominal step where x is supplied at run-time 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: `numdifftools.limits._Limit`

Compute limit of a function at a given point

#### Parameters

**fun** [callable] function `fun(z, *args, **kws)` to compute the limit for  $z \rightarrow z_0$ . 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  $z \rightarrow z_0$

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

**error estimate: ndarray** 95 % uncertainty estimate around the limit, such that  $\text{abs}(\text{limit\_fz} - \lim_{z \rightarrow z_0} f(z)) < \text{error\_estimate}$

**final\_step: ndarray** final step used in approximation

#### Notes

*Limit* computes the limit of a given function at a specified point,  $z_0$ . 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  $z_0$ .  $z_0$  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  $z_0$  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  $z_0$  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  $1/(1-\exp(2z))$  has a pole at  $z = 0$ . The residue is given by the limit of  $z \cdot \text{fun}(z)$  as  $z \rightarrow 0$ . Here, that residue should be -0.5.

```
>>> def h(z): return -z/(np.exp(2*z)-1)
>>> 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  $z^2 \cdot \text{fun}(z)$  as  $z \rightarrow 0$ .

```
>>> 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.exp(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*, \*\**kws*)

Return  $\lim_{z \rightarrow x} f(z)$

**class Residue** (*f*, *step=None*, *method='above'*, *order=None*, *pole\_order=1*, *full\_output=False*, *\*\*options*)

Bases: `numdifftools.limits.Limit` (page 103)

Compute residue of a function at a given point

#### Parameters

**fun** [callable] function `fun(z, *args, **kws)` to compute the Residue at  $z=z_0$ . 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  $z_0$ .

**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  $f(z)(z-z_0)^{pole\_order}$  as  $z \rightarrow z_0$  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  $abs(res\_fz - \lim_{z \rightarrow z_0} f(z)(z-z_0)^{pole\_order}) < error\_estimate$  Large uncertainties here suggest that the wrong order pole was specified for  $f(z_0)$ .

**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.expml(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: object62
```

Creates an instance of a Bicomplex object.  $\zeta = z_1 + j \cdot z_2$ , where  $z_1$  and  $z_2$  are complex numbers.

```
arccos ()
```

```
arccosh ()
```

```
arcsin ()
```

```
arcsinh ()
```

```
arctan ()
```

```
arctanh ()
```

```
arg_c ()
```

```
arg_clp ()
```

```
static asarray (other)
```

```
conjugate ()
```

```
cos ()
```

```
cosh ()
```

```
cot ()
```

```
coth ()
```

```
csc ()
```

```
csch ()
```

```
dot (other)
```

```
exp ()
```

```
exp2 ()
```

---

<sup>62</sup> <https://docs.python.org/3.8/library/functions.html#object>



`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)`

## 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 Algorithmic 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. Algorithmic 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://en.wikipedia.org/wiki/Automatic_differentiation)

<https://pythonhosted.org/algopy/index.html>

**class Derivative** (*fun, n=1, method='forward', full\_output=False*)

Bases: numdifftools.nd\_algopy.\_Derivative

Calculate n-th derivative with Algorithmic Differentiation method

#### Parameters

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

**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 109)[Hessdiag](#) (page 111)[Hessian](#) (page 112)[Jacobian](#) (page 113)

## 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**class Gradient** (*fun*, *n=1*, *method='forward'*, *full\_output=False*)

Bases: numdifftools.nd\_algopy.\_Derivative

Calculate Gradient with Algorithmic Differentiation method

### Parameters

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

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

### Returns

**grad:** array gradient

See also:

[\*Derivative\*](#) (page 108)

[\*Jacobian\*](#) (page 113)

[\*Hessdiag\*](#) (page 111)

[\*Hessian\*](#) (page 112)

### 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](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  $\sin(x-y) + y \cdot \exp(x)$

```
>>> 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

<b><code>__call__</code></b> : callable with the following parameters:	<code>x</code> : array_like value at which function derivative is evaluated <code>args</code> : tuple Arguments for function <i>fun</i> . <code>kwds</code> : dict Keyword arguments for function <i>fun</i> .
--	--

**class Hessdiag** (*f*, *method*='forward', *full\_output*=False)

Bases: [numdifftools.nd\\_algopy.Hessian](#) (page 112)

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 108)

[Gradient](#) (page 109)

[Jacobian](#) (page 113)

[Hessian](#) (page 112)

## 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**class** **Hessian** (*f*, *method*='forward', *full\_output*=False)

Bases: numdifftools.nd\_algopy.\_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 108)

[\*Gradient\*](#) (page 109)

[\*Jacobian\*](#) (page 113)

[\*Hessdiag\*](#) (page 111)

## 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](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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**class** `Jacobian` (*fun*, *n=1*, *method='forward'*, *full\_output=False*)

Bases: `numdifftools.nd_algopy.Gradient` (page 109)

Calculate Jacobian with Algorithmic Differentiation method

### Parameters

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

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

### Returns

**jacob: array** Jacobian

See also:

[Derivative](#) (page 108)

[Gradient](#) (page 109)

[Hessdiag](#) (page 111)

[Hessian](#) (page 112)

## 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](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.]])
```

```
>>> 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

<b><code>__call__</code></b> : callable with the following parameters:	x: array_like value at which function derivative is evaluated args: tuple Arguments for function <i>fun</i> . kwds: dict Keyword arguments for function <i>fun</i> .
--	--

**class Taylor** (*fun*, *n=1*)

Bases: `object`<sup>63</sup>

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 coefficients to compute.

### Returns

**coefs**: ndarray array of taylor coefficients

## Examples

Compute the first 6 taylor coefficients  $1 + 2z + 3z^2$  expanded round  $z_0 = 0$ :

```

>>> 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.

<sup>63</sup> <https://docs.python.org/3.8/library/functions.html#object>

**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 108)

[Gradient](#) (page 109)

#### 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
```

### 5.2.9 numdifftools.nd\_scipy module

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

Bases: [numdifftools.nd\\_scipy.Jacobian](#) (page 117)

Calculate Gradient with finite difference approximation

#### Parameters

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

**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 117)

## 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: numdifftools.nd\_scipy.\_Common

Calculate Jacobian with finite difference approximation

### Parameters

**fun** [function] function of one array  $\text{fun}(x, *args, **kws)$

**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: [numdifftools.nd\\_statsmodels.Jacobian](#) (page 119)

Calculate Gradient with finite difference approximation

#### Parameters

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

**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 118), [Jacobian](#) (page 119)

#### 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: numdifftools.nd\_statsmodels.\_Common

Calculate Hessian with finite difference approximation

#### Parameters

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

**step** [float, optional] Stepsize, if None, optimal stepsize is used, i.e.,  $x * \_EPS^{**}(1/3)$  for method=='forward', *complex* or *central*  $2 * \_EPS^{**}(1/4)$  for method=='central'.

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

See also:

[Jacobian](#) (page 119), [Gradient](#) (page 118)

#### 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: numdifftools.nd\_statsmodels.\_Common

Calculate Jacobian with finite difference approximation

#### Parameters

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

**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  $x_k \times \text{nobs} \times x_k$ . 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  $\text{EPS} \times x$ . 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  $O(\text{epsilon}^{**2})$ , 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`<sup>64</sup>

Generates a sequence of steps of decreasing magnitude

**where**  $\text{steps} = \text{base\_step} * \text{step\_ratio} ** (-i + \text{offset})$

for  $i=0, 1, \dots, \text{num\_steps}-1$ .

### 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

<sup>64</sup> <https://docs.python.org/3.8/library/functions.html#object>

## 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: [numdifftools.step\\_generators.BasicMaxStepGenerator](#) (page 121)

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: [numdifftools.step\\_generators.MinStepGenerator](#) (page 123)

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  $\text{EPS}^{**}(1/\text{scale})$

**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 run-time 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`<sup>65</sup>

Generates a sequence of steps

**where**  $\text{steps} = \text{step\_nom} * \text{base\_step} * \text{step\_ratio} ** (i + \text{offset})$

for  $i = \text{num\_steps}-1, \dots, 1, 0$ .

### Parameters

**base\_step** [float, array-like, optional] Defines the minimum step, if None, the value is set to  $\text{EPS} ** (1/\text{scale})$

**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  $\text{min\_num\_steps} + \text{num\_extrap}$ ] defines number of steps generated. It should be larger than  $\text{min\_num\_steps} = (n + \text{order} - 1) / \text{fact}$  where fact is 1, 2 or 4 depending on differentiation method used.

**step\_nom** [default  $\text{maximum}(\log(\exp(1)+|x|), 1)$ ] Nominal step where  $x$  is supplied at run-time 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  $\text{base\_step} = \text{EPS} ** (1. / \text{scale})$

### **get\_nominal\_step** (*x=None*)

Return nominal step

<sup>65</sup> <https://docs.python.org/3.8/library/functions.html#object>

**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.

## 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 continuous 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 the 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 file 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 XXXDifferencedFunctions 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 quotes 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 confestest.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.
- missing 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 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 unnecessary parenthesis. 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 sonarcube 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 fornborg\_weights to fornborg.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 unnecessary 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 formatting
- Migrated % string formatting

### **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 quantifcode
- 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 issue #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.
- Restructured 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  $\max(\text{abs}(x_0), 0.2)$  to  $\max(\log_2(\text{abs}(x_0)), 0.2)$ .
- 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

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## **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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