

1 Introduction

This report discusses development of the package designed to implement automatic differentiation using dual numbers in Python.

2 Repository

2.1 Structure

Good practice suggests the following directory structure:

```
dual_autodiff
├── dual_autodiff
│   ├── __init__.py
│   └── dual.py
├── tests
│   └── test_dual.py
├── docs
│   └── ...
├── build
│   └── ...
├── source
│   └── ...
├── pyproject.toml
├── setup.py
├── README.md
├── Makefile
└── LICENSE
```

2.2 Project configuration

The following is the contents of the `pyproject.toml` file.

Listing 1: `pyproject.toml`

```
[build-system]
requires = ["setuptools", "wheel", "setuptools_scm"]
build-backend = "setuptools.build_meta"

[project]
name = "dual_autodiff"
version = "0.0.1"
description = "A Python package for automatic
    differentiation using dual numbers."
readme = "README.md"
requires-python = ">=3.10"
license = { file = "LICENSE" }
```

```

authors = [
    { name = "Laura Just Fung", email = "lj441@cam.ac.uk"
      }
]

dependencies = [
    "numpy"
]

[tool.setuptools_scm]
write_to = "dual_autodiff/version.py"
version_scheme = "post-release"
local_scheme = "no-local-version"

[tool.setuptools.packages.find]
where = ["."]

[project.urls]
Homepage = "https://github.com/ljf441/dual_autodiff"
Issues = "https://github.com/ljf441/dual_autodiff/issues"

```

3 Implementation

3.1 Dual class

The Dual class is defined and initialised like so:

Listing 2: Dual class

```

class Dual:
    def __init__(self, real, dual):
        self.real = real
        self.dual = dual

```

A dual number can be initialised as follows:

CELL 02
<pre> # initialise dual number x = df.Dual(2, 1) print(f"x.real = {x.real}, x.dual = {x.dual}") </pre> <hr/> <pre> x.real = 2, x.dual = 1 </pre>

And it produces the following output when printed:

CELL 03
<pre># printing dual number print(x)</pre>
Dual(real=2, dual=1)

3.2 Arithmetic operations

Arithmetic operations include: addition, subtraction, multiplication, and division. The Dual class allows for these arithmetic operations performed over dual numbers as well as real numbers. An example is as follows:

CELL 04
<pre># basic arithmetic operations x = df.Dual(2, 1) y = df.Dual(3, 2) print(f"x + y = {x + y}") print(f"x - y = {x - y}") print(f"x * y = {x * y}") print(f"x / y = {x / y}")</pre>
<pre>x + y = Dual(real=5, dual=3) x - y = Dual(real=-1, dual=-1) x * y = Dual(real=6, dual=7) x / y = Dual(real=0.6666666666666666, dual=-0.25)</pre>

3.3 Trigonometric operations

Trigonometric operations include: sine, cosine, and tangent. The Dual class allows for these trigonometric operations performed over dual numbers. An example is as follows:

CELL 05
<pre># trigonometric operations print(f"sin(x) = {x.sin()}") print(f"cos(x) = {x.cos()}") print(f"tan(x) = {x.tan()}")</pre>
<pre>sin(x) = Dual(real=0.9092974268256817, dual=-0.4161468365471424) cos(x) = Dual(real=-0.4161468365471424, dual=-0.9092974268256817) tan(x) = Dual(real=-2.185039863261519, dual=5.774399204041917)</pre>

3.4 Other operations

Other implemented operations that the Dual class allows for over dual numbers are: natural logarithm, exponential, power. An example is as follows:

CELL 06

```
# the natural logarithm and exponential

print(f"log(x) = {x.log()}")
print(f"exp(x) = {x.exp()}")

-----

log(x) = Dual(real=0.6931471805599453, dual=0.5)
exp(x) = Dual(real=7.38905609893065, dual=7.38905609893065)
```

CELL 07

```
# powers

print(f"x**y = {x**y}")

-----

x**y = Dual(real=8, dual=35.090354888959126)
```

4 Package

The package is installable with `pip install -e .` from the root project folder. The package is importable with `import dual_autodf as df`.

5 Differentiation

Consider the function $f(x) = \log \sin x + x^2 \cos x$ where $x = 1.5$. The derivative can be easily calculated using `dual_autodiff`:

CELL 08

```
# automatic differentiation

#initialise x = 1.5, with x.dual = 1 to allow for differentiation
x = df.Dual(1.5, 1)

function = x.sin().log() + x**2 * x.cos() #f(x) = log(sin(x)) + x^2 * cos(x)

print(f"log(sin(x)) + x^2 cos(x) = {function.real}")
print(f"d/dx(log(sin(x)) + x^2 cos(x)) = {function.dual}")

-----

log(sin(x)) + x^2 cos(x) = 0.15665054756073515
d/dx(log(sin(x)) + x^2 cos(x)) = -1.9612372705533612
```

6 Test suite