Introduction

Describe the problem the software solves and why it's important to solve that problem.

- Our software package, *ad-AHJZ*, computes gradients by leveraging the technique of automatic differentiation. Before we can understand automatic differentiation, we must first describe and motivate the importance of differentiation itself. Derivatives are vital to quantifying the change that's occurring over a relationship between multiple factors. Finding the derivative of a function measures the sensitivity to change of a function value with respect to a change in its input argument. Derivatives generalize across multiple scenarios and are well defined for both scalar inputs and outputs, as well as vector inputs and outputs. Derivatives are not only essential in calculus applications like numerically solving differential equations and optimizing and solving linear systems, but are useful in many real world, scientific settings. For example, in finance they help analyze the change regarding the profit/loss for a business or finding the minimum amount of material to construct a building. In physics, they help calculate the speed and distance of a moving object. Derivatives are crucial to understanding how such relationships move and change.
- To perform differentiation, two different approaches are solving the task symbolically or numerically computing the derivatives. Symbolic differentiation yields accurate answers, however depending on the complexity of the function, it could be expensive to evaluate and result in inefficient code. On the other hand, numerically computing derivatives is less expensive, however it suffers from potential issues with numerical stability and a loss of accuracy.
- Our software package, *ad-AHJZ*, overcomes the shortcomings of both the symbolic and numerical approach. Our package uses automatic differentiation which is less costly than symbolic differentiation, but evaluates derivatives at machine precision. The technique leverages both forward mode and backward mode and evaluates each step with the results of previous computations or values. As a result of this, automatic differentiation avoids finding the entire analytical expresssion to compute the derivative and is hence iteratively evaluating a gradient based on input values. Thus, based on these key advantages, our library implements and performs forward mode automatic differentiation to efficiently and accurately compute derivatives.

Background

Describe (briefly) the mathematical background and concepts as you see fit.

Part 1: Chain Rule

The underlying motivation of automatic differentiation is the Chain Rule that enables us to decompose a complex derivative into a set of derivatives involving elementary functions of which we know explicit forms.

We will first introduce the case of 1-D input and generalize it to multidimensional inputs.

One-dimensional (scalar) Input: Suppose we have a function $f(y(t))$ and we want to compute the derivative of f with respect to t. This derivative is given by:

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial t}$$

Before introducing vector inputs, let's first take a look at the gradient operator ∇

That is, for y: $\mathbb{R}^n \rightarrow \mathbb{R}$, its gradient ∇y: $\mathbb{R}^n \rightarrow \mathbb{R}^n$ is defined at the point $x = (x_1, \ldots, x_n)$ in n-dimensional space as the vector:

$$\nabla y(x) = \begin{bmatrix} \frac{\partial y}{\partial x_1}(x) \\ \vdots \\ \frac{\partial y}{\partial x_n}(x) \end{bmatrix}$$

Multi-dimensional (vector) Inputs: Suppose we have a function $f(y_1(x), \ldots, y_n(x))$ and we want to compute the derivative of f with respect to x. This derivative is given by:

$$\nabla f_x = \sum_{i=1}^{n} \frac{\partial f}{\partial y_i}\nabla y_i(x)$$

We will introduce direction vector p later to retrieve the derivative with respect to each y_i.

Part 2: Jacobian-vector Product

The Jacobian-vector product is equivalent to the tangent trace in direction p if we input the same direction vector p:

$D_p v = Jp$

Part 3: Seed Vector

Seed vectors provide an efficient way to retrieve every element in a Jacobian matrix and also recover the full Jacobian in high dimensions.

Scenario: Seed vectors often come into play when we want to find $\frac{\partial f_i}{\partial x_j}$, which corresponds to the i, j element of the Jacobian matrix.

Procedure: In high dimension automatic differentiation, we will apply seed vectors at the end of the evaluation trace where we have recursively calculated the explicit forms of tangent trace of f_is and then multiply each of them by the indicator vector p_j where the j-th element of the p vector is 1.

Part 4: Evaluation (Forward) Trace

Definition: Suppose x = $\begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$, we defined $v_{k-m} = x_k$ for $k = 1, 2, \ldots, m$ in the evaluation trace.

Motivation: The evaluation trace introduces intermediate results v_{k-m} of elementary operations to track the differentiation.

Consider the function $f(x) : \mathbb{R}^2 \rightarrow \mathbb{R}$:

$f(x) = log(x_1) + sin(x_1 + x_2)$

We want to evaluate the gradient ∇f at the point $x = \begin{bmatrix} 7 \\ 4 \end{bmatrix}$. Computing the gradient manually:

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{x_1} + \cos(x_1 + x_2) \\ \cos(x_1 + x_2) \end{bmatrix} = \begin{bmatrix} \frac{1}{7} + \cos(11) \\ \cos(11) \end{bmatrix}$$

Forward primal trace	Forward tangent trace	Pass with p = $[0,1]^T$	Pass with p = $[1,0]^T$
$v_{-1} = x_1$	p_1	1	0
$v_0 = x_2$	p_2	0	1
$v_1 = v_{-1} + v_0$	$D_p v_{-1} + D_p v_0$	1	1
$v_2 = sin(v_1)$	$\cos(v_1) D_p v_1$	$\cos(11)$	$\cos(11)$
$v_3 = log(v_{-1})$	$\frac{1}{v_{-1}} D_p v_{-1}$	$\frac{1}{7}$	0
$v_4 = v_3 + v_2$	$D_p v_3 + D_p v_2$	$\frac{1}{7} + \cos(11)$	$\cos(11)$

$D_p v_{-1} = \nabla v_{-1}^T p = (\frac{\partial v_{-1}}{\partial x_1}\nabla x_1)^T p = (\nabla x_1)^T p = p_1$

$D_p v_0 = \nabla v_0^T p = (\frac{\partial v_0}{\partial x_2}\nabla x_2)^T p = (\nabla x_2)^T p = p_2$

$D_p v_1 = \nabla v_1^T p = (\frac{\partial v_1}{\partial v_{-1}}\nabla v_{-1} + \frac{\partial v_1}{\partial v_0}\nabla v_0)^T p = (\nabla v_{-1} + \nabla v_0)^T p = D_p v_{-1} + D_p v_0$

$D_p v_2 = \nabla v_2^T p = (\frac{\partial v_2}{\partial v_1}\nabla v_1)^T p = \cos(v_1)(\nabla v_1)^T p = \cos(v_1) D_p v_1$

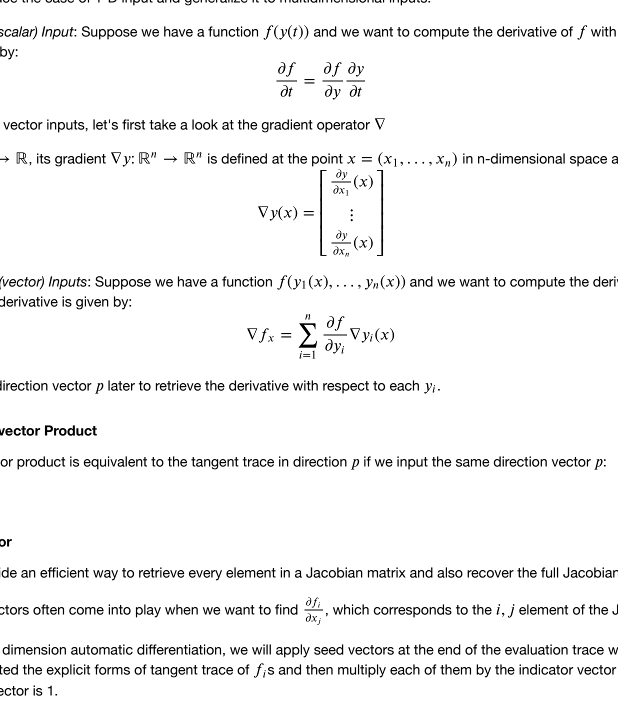
$D_p v_3 = \nabla v_3^T p = (\frac{\partial v_3}{\partial v_{-1}}\nabla v_{-1})^T p = \frac{1}{v_{-1}}(\nabla v_{-1})^T p = \frac{1}{v_{-1}} D_p v_{-1}$

$D_p v_4 = \nabla v_4^T p = (\frac{\partial v_4}{\partial v_3}\nabla v_3 + \frac{\partial v_4}{\partial v_2}\nabla v_2)^T p = (\nabla v_3 + \nabla v_2)^T p = D_p v_3 + D_p v_2$

Part 5: Computation (Forward) Graph

We have connected each v_{k-m} to a node in a graph for a visualization of the ordering of operations.

From the above example, its computational graph is given by:



Part 6: Computing the Derivative

Let's generalize our findings:

From the table, we retrieved a pattern as below:

$$D_p v_j = (\nabla v_j)^T p = (\sum_{i<j} \frac{\partial v_j}{\partial v_i}\nabla v_i)^T p = \sum_{i<j} \frac{\partial v_j}{\partial v_i}(\nabla v_i)^T p = \sum_{i<j} \frac{\partial v_j}{\partial v_i} D_p v_i$$

Higher dimension: We recursively apply the same technique introduced above to each entry of the vector valued function *f*.

Part 7: Efficiency of Forward Mode

Forward mode is efficient in the sense that it does not need to store the parent node, which is different from reverse mode (see below) where the whole computational graph must be stored.

Part 8: Reverse Mode

The mechanism of reverse mode is defined as the following:

Step 1: Calculate $\frac{\partial f}{\partial v_j}$

Step 2: Calculate $\frac{\partial v_j}{\partial v_i}$ where v_i is the immediate predecessor of v_j

Step 3: Multiply the result obtained in step 1 and step 2, which results in the following: $\frac{\partial f}{\partial v_j}\frac{\partial v_j}{\partial v_i}$

Part 9: Dual Number

Naively: We define a dual number $d_i = v_i + \delta_i$ where $\delta_i = D_p v_i \epsilon$ that satisfies $\epsilon^2 = 0$

A k-th differentiable function f can be written as:

$f(d_i) = f(v_i + \delta_i) = f(v_i) + f'(v_i)\delta_i + \frac{f''(v_i)}{2!}\delta_i^2 + \ldots + \frac{f^k(v_i)}{k!}(\zeta - v_i)^k$ for some $\zeta \in (v_i, v_i + \delta_i)$ by Taylor expansion.

Now we substitute the definition of δ_i back into the above expansion and use the fact that all higher terms go to 0 assuming $\epsilon^2 = 0$. We will have the following:

$f(d_i) = f(v_i) + f'(v_i) D_p v_i \epsilon$

Advantage: Operations on Dual Number pertain to the form of Taylor expansion, which makes the implementation easier to retrieve the value and derivative.

Consider the following example:

$$d_i = v_i + D_p v_i \epsilon$$
$$f(d_i) = d_i^2 = v_i^2 + 2v_i D_p v_i \epsilon + D_p v_i^2 \epsilon^2 = v_i^2 + 2v_i D_p v_i \epsilon$$

where v_i^2 refers to the value and $2v_i D_p v_i$ refers to the derivative.

More specifically, v_i^2 corresponds to $f(v_i)$, $2v_i$ corresponds to $f'(v_i)$, and $D_p v_i$ is just $D_p v_i$.

How to Use ad-AHJZ

How does a user interact with your package? What should they import? How can they instantiate AD objects?

1. Installing the package:

We note that we have two options for installing our package. The first option (1a. below) is to download the package from our Github repository. The second option (1b-i and 1b-ii. below) is to install the package from PyPI.

- 1a. (Option 1 for installation) User can download the package via our GitHub repository:

```
# Create a virtual environment as shown in 1b-i or 1b-ii below

# Navigate to the desired folder and clone the repo from
# https://github.com/cs107-AHJZ/cs107-FinalProject.git
git clone https://github.com/cs107-AHJZ/cs107-FinalProject.git
cd cs107-FinalProject
pip install -r requirements.txt
# From cs107-FinalProject move the package folder ad_AHJZ into
# the desired folder with your python file
```

- 1b-i. (Option 2 for installation) User can install the package and its dependencies using the "venv" virtual environment:

```
# Create a directory to store your virtual environment(s)
mkdir ~/.virtualenvs
python3 -m venv ~/.virtualenvs/env_name
# Activate your env_name virtual environment
source ~/.virtualenvs/env_name/bin/activate
# Install the package
python3 -m pip install ad-AHJZ
# Create a Python file to use the package in
echo >'file_name'.py
```

- 1b-ii. (Option 3 for installation) User can install the package and its dependencies using the "conda" virtual environment:

```
# Create a directory to store your virtual environment(s)
mkdir 'directory_name_for_virtual_environment'
cd 'directory_name_for_virtual_environment'
conda create -n 'env_name' python=3.7 anaconda
# Activate your env_name virtual environment
source activate env_name
# Install the package
python3 -m pip install ad-AHJZ
# Create a Python file to use the package in
echo >'file_name'.py
```

2. Importing the package:

- 2a-i. (Option 1 - for Github download) User imports package and dependencies into the desired python file with the following line:

```
from ad_AHJZ.forward_mode import forward_mode
import numpy as np
```

- 2a-ii. (Option 2 - for PyPi installation) User imports package and dependencies into the desired python file with the following line:

```
from ad_AHJZ import forward_mode
import numpy as np
```

3. Calling/Using package modules:

- 3a. Using the class *forward_mode()* create an automatic differentiation object that can use either a scalar or vector input to obtain both the function value and derivative. Below are examples using a scalar input and a vector input:
- 3b. Example of *forward_mode()* using a scalar input:

```
# Define desired evaluation value (scalar)
x = 0.5
# Define a simple function:
f_x = lambda x: np.sin(x) + 2 * x
# Create a forward_mode() object using the defined
# values x, f_x from above
fm = forward_mode(x, f_x)

# Option 1: retrieve both the function value
# and the derivative using get_function_value_and_jacobian()
x, x_der = fm.get_function_value_and_jacobian()
print(x, x_der)
>>> 1.479425538604203
    [2.87758256]

# Option 2: retrieve only the function value
# using get_function_value()
x_value = fm.get_function_value()
print(x_value)
>>> 1.479425538604203

# Option 3: retrieve only the function derivative
# using get_jacobian()
x_derivative = fm.get_jacobian()
print(x_derivative)
>>> [2.87758256]
```

- 3c. Example of *forward_mode()* using a vector input:

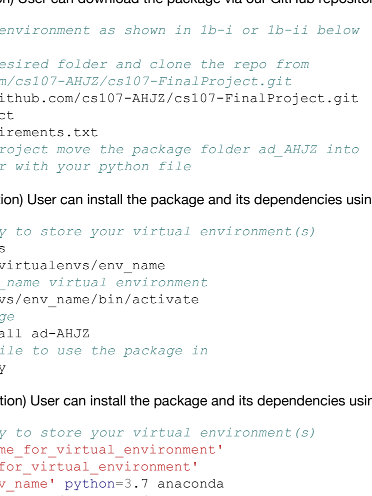
```
# Define desired evaluation value (vector)
multi_input = [0.5, 1]
# Define a simple function:
f_xy = lambda x, y: np.sin(x) + 2 * y
# Create a forward_mode() object using the
# defined values multi_input, f_xy from above
fm = forward_mode(multi_input, f_xy)

# Option 1: retrieve both the function value and
# the jacobian using get_function_value_and_jacobian()
multi_xy, multi_xy_der = fm.get_function_value_and_jacobian()
print(multi_xy, multi_xy_der)
>>> 2.479425538604203
    [0.87758256 2.        ]

# option 2: retrieve only the function value
# using get_function_value()
multi_xy_value = fm.get_function_value()
print(multi_xy_value)
>>> 2.479425538604203

# option 3: retrieve only the function
# jacobian using get_jacobian()
multi_xy_derivative = fm.get_jacobian()
print(multi_xy_derivative)
>>> [0.87758256 2.        ]
```

Software Organization

Discuss how you organized your software package.

1. Directory Structure:

- 1a. We include our project directory structure in the image below. Our package is called *ad-AHJZ*, where our code for automatic differentiation lies within "ad_AHJZ", our milestone documentation lies within "docs", all unit testing files are located in "testing", and the root of the directory holds our readme.md, license, .gitignore, .coveragerc, codecov.yml, codecov, setup.cfg, setup.py, and requirements.txt file.
- 1b. Directory structure layout:



```
└───cs107-FinalProject
    │   .coveragerc
    │   .gitignore
    │   codecov
    │   codecov.yml
    │   LICENSE.txt
    │   README.md
    │   requirements.txt
    │   setup.cfg
    │   setup.py
    │
    ├───ad_AHJZ
    │       forward_mode.py
    │       val_derv.py
    │       __init__.py
    │
    ├───docs
    │       auto_diff_project_directory_structure.png
    │       computational_graph.png
    │       milestone1.ipynb
    │       milestone2.ipynb
    │       milestone2_progress.ipynb
    │
    └───tests
            test_forward_mode.py
            test_val_derv.py
            __init__.py
```

2. Modules:

- 2a. *val_derv.py*: This file contains the class definition of a value/derivative object. It contains methods to initialize the object, set and get the function and derivative value of the object, overload elementary operations, and define elementary functions. Specifically, we overload addition, multiplication, division, negation, power, reverse addition, reverse subtraction, reverse multiplication, and reverse division. Finally, we include elementary functions on these objects including 'sqrt', 'log', 'exp', 'sin', 'cos', 'tan', 'sinh', 'cosh', 'tanh', 'arcsin', 'arccos', and 'arctan'. This is not a file which the user will interact with.
- 2b. *forward_mode.py*: This file contains the class definition to perform forward mode automatic differentiation. This is the module which the user will interact with to compute function values and derivatives using forward mode. Specifically, the user will create forward mode objects using the function they are interested in computing the derivative of and the point or vector at which to evaluate the function. Next, after initialization, they can make use of *get_function_value()* to retrieve function values, *get_jacobian()* to retrieve derivative values, and *get_function_value_jacobian()* to retrieve both the function and derivative values.
- 2c. *init.py*: This file contains information relevant to how each of the modules associated with our package ad-AHJZ interact with one another.
- 2d. *reverse_mode.py*: This file (once implemented) will contain the class definition to perform reverse mode automatic differentiation. This is the module which the user will interact with to compute function values and derivatives using reverse mode. Specifically, the user will create reverse mode objects using the function they are interested in computing the derivative of and the point or vector at which to evaluate the function. Next, after initialization, the user will call the methods on these objects to retrieve function and derivative values.

3. Test Suite Location:

- 3a. The test suite live in the "testing" directory which is a subdirectory found off the root directory (see 1. Directory Structure). The "testing" directory contains all unit tests and integration tests.
- 3b. Our testing suite is built using Python's unittest framework. We have two files for testing, which are *test_val_derv.py* and *test_forward_mode.py*. The first file tests scalar inputs for *val_derv.py* to ensure all overloaded operations and elementary functions are implemented correctly and the second file tests *forward_mode.py* to ensure the automatic differentiation is performed correctly in terms of computing function values and derivatives. We run our tests by running "coverage run -m unittest discover -s tests/" in the root directory.
- 3c. To ensure our testing procedure has complete code coverage, we leverage CodeCov. CodeCov enables us to quickly understand which lines are being executed in our test cases. We directly upload our coverage reports to CodeCov through the use of a bash script and the .coveragerc, codecov, and codecov.yml files.

4. Package Distribution and Installation:

- 4a. Our package is distributed via PyPI. We have uploaded the package to PyPI using the setup.py and setup.cfg files which contain relevant information about our package as well as the version number, associated dependencies, and the license.
- 4b. A user can install our package from PyPI by creating a virtual environment as shown in *Installing the package* in **How to Use ad-AHJZ**. Once a virtual environment has been created, the user can install our package by running the following lines:

```
python3 -m pip install ad-AHJZ
python3 -m pip install -r requirements.txt
```

- 4c: After installing our package, a user can import it into their desired python file and use it by including the following two lines at the top of their file:

```
from ad_AHJZ import forward_mode
import numpy as np
```

5. Package Dependencies

- 5a. The only library dependency our package relies on is numpy. We designed our software in this manner to ensure that we are not creating multiple external dependencies and thereby increase our software's reliability.

Implementation

Discuss how you implemented the forward mode of automatic differentiation.

1. Core Data Structure:

- 1a. Our primary core data structure is the numpy array, which we use to store both the variable list and the function list. Then using the methods within the *forward_method* class we compute the jacobian and function value storing those values or arrays, depending on the input, in a tuple.

2. Classes:

- 2a. *Val Derv:* The class that creates our *val_derv* object. This object has two attributes: the value and the derivative seed, which can be defined at instantiation. This object will be used with the elementary function methods to calculate the value, and the dual number at a particular state of the primal or tangent trace.
- 2b. *Forward Mode:* The class that creates a *forward_mode* object. This object has two attributes: the variable list and the function list, which can be defined at instantiation. Both attributes can be in either the scalar or vector form, and will be used to find either the function value, the jacobian, or both.
- 2c. *Reverse Mode* (extension module): The class that creates a *reverse_mode* object. This object has two attributes: the variable list and the function list, which can be defined at instantiation. Both attributes can be in either the scalar or vector form, and will be used to find either the function value, the jacobian, or both.

3. Methods:

- 3a. *Val Derv* Methods: Below we include a list of all methods in our *Val Derv* class along with their description:

Method	Description
`__init__`	Constructor for the `val_derv` class
`__repr__`	Operator overloading for `val_derv` object string representations
`@property val`	Gets the value attribute of `val_derv` object
`@property derv`	Gets the derivative attribute of `val_derv` object
`@val.setter val`	Sets the value attribute of `val_derv` object
`@derv.setter derv`	Sets the derivative attribute of `val_derv` object
`__add__`	Compute the value and derivative of the addition operation
`__mul__`	Compute the value and derivative of the multiplication operation
`__truediv__`	Compute the value and derivative of the division operation
`__neg__`	Compute the value and derivative of the negation operation
`__pow__`	Compute the value and derivative of the power operation
`__radd__`	Compute the value and derivative of the addition operation
`__rsub__`	Compute the value and derivative of the subtraction operation
`__rmul__`	Compute the value and derivative of the multiplication operation
`__rtruediv__`	Compute the value and derivative of the division operation
`__rpow__`	Compute the value and derivative of the power operation
`sqrt`	Compute the value and derivative of the square root function
`log`	Compute the value and derivative of logarithmic function (Default base 10)
`exp`	Compute the value and derivative of exponential function
`sin`	Compute the value and derivative of the sine function
`cos`	Compute the value and derivative of the cosine function
`tan`	Compute the value and derivative of the tangent function
`sinh`	Compute the value and derivative of the hyperbolic sine function
`cosh`	Compute the value and derivative of the hyperbolic cosine function
`tanh`	Compute the value and derivative of the hyperbolic tangent function
`arcsin`	Compute the value and derivative of the inverse sine function
`arccos`	Compute the value and derivative of the inverse cosine function
`arctan`	Compute the value and derivative of the inverse tangent function

- 3b. *Forward Mode* Methods: Below we include a list of all methods in our *Forward Mode* class along with their description:

Method	Description
`__init__`	Constructor for the `forward_mode` class
`get_function_value`	Extracts function value from `get_function_value_and_jacobian`
`get_jacobian`	Extracts jacobian matrix from `get_function_value_and_jacobian`
`get_function_value_and_jacobian`	Calculates the function value and jacobian of a user input function

- 3c. *Reverse Mode (Potential Methods)* Methods: Below we include a list of all methods that we plan to include in our *Reverse Mode* class along with their description:

Method	Description
`__init__`	Constructor for the `reverse_mode` class
`get_function_value`	Extracts function value from `get_function_value_and_jacobian`
`get_jacobian`	Extracts jacobian matrix from `get_function_value_and_jacobian`
`get_function_value_and_jacobian`	Calculates the function value and jacobian of a user input function

4. External Dependencies:

- 4a. To be viewed as a near stand alone software package, to improve adoption, and increase efficiency, we chose to only employ a single external library, numpy. We've used the numpy library to create our data structure for the computational graph and perform computations outside of those we created in our *val_derv* class.

5. Dealing With Elementary Functions

- 5a. As listed above, within the *val_derv* class we've overloaded the simple arithmetic functions (addition, subtraction, multiplication, division, negation, and power) to calculate both the value and the dual number. We've also defined our own elementary functions, such as sin(x) and sqrt(x) (see **Methods** above for full list) to compute the value and the derivative. This module generalizes each of the functions in order to handle both scalar and vector inputs. Each method also indicates errors specific to the types of possible invalid inputs. The output is a tuple of both the function value and the derivative, which is used in the *forward_mode* and (eventually) the *reverse_mode*.
- 5b. Below are examples of how the user would implement *sin* and *sqrt*, both of which work with scalar or vector input values, within the *val_derv* class:

```
# sqrt of variable with scalar derivative
x = val_derv(1, 1)
print(x.sqrt())
>>>Values:1.0, Derivatives:0.5
```

```
# sqrt of variable with vector derivative
x = val_derv(1, np.array([1, 0]))
print(x.sqrt())
>>>Values:1.0, Derivatives:[0.5 0. ]
```

```
# sin of variable with scalar derivative
x = val_derv(0, 1)
print(x.sin())
>>>Values:0.0, Derivatives:1.0
```

```
# sin of variable with vector derivative
x = val_derv(0, np.array([1, 0]))
print(x.sin())
>>> Values:0.0, Derivatives:[1. 0.]
```

6. Next Steps

- 6a. As alluded to earlier, our next steps will be to implement reverse mode, similar to our forward mode class structure. The reverse mode class will employ a dictionary data structure to store the computational graph and will depend on our *val_derv* class to compute the values and derivatives for the elementary functions. We will also expand the number of elementary functions our package will be able to calculate the value and derivative of to include functions such as less than and greater than. Finally, we will look towards implementing an optimized version of our forward class to improve efficiency, while using complex inputs.

Licensing

Briefly motivate your license choice

Our *ad-AHJZ* package is licensed under the GNU General Public License v3.0. This free software license allows users to do just about anything they want with our project, except distribute closed source versions. This means that any improved versions of our package that individuals seek to release must also be free software. We find it essential to allow users to help each other share their bug fixes and improvements with other users. Our hope is that users of this package continually find ways to improve it and share these improvements within the broader scientific community that uses automatic differentation.

Future Features

Discuss how you plan on expanding the automatic differentiation package to include additional features.

1. What kinds of things do you want to implement next?

- One key area which we would like to expand or implement next in our package is the support for more elementary functions and operations in *val_derv.py*. Currently, we provide users with twenty-two options which overload basic arithmetic operations along with the trigonometric functions. However, for advanced users that could use our package to solve complex computational problems, we believe that providing support for even more complex functions and operations could prove useful in providing generalizability.
- Another key capability we would like to implement is providing reverse mode automatic differentiation. Providing a class analogous to forward mode, but which instead simulates reverse mode is important due to the computational efficiency we can provide our users with. Compared to forward mode, reverse mode has a significantly smaller arithmetic operation count for mappings of the form $f(x) : R^n \rightarrow R^m$ when $n >> m$. Users that choose to use our library to tackle large-scale machine learning tasks would require efficient and reliable differentiation and so it is critical that our package provide users with this option to carry out automatic differentiation using either method. We plan on creating a reverse mode class which will serve as our primary extension module for this project.
- We would also like to implement an enhanced version of forward mode, time permitting. We believe that the reverse mode implementation mentioned above will certainly provide computational efficiency for users that want access to fast differentiation for mappings of the form $f(x) : R^n \rightarrow R^m$ when $n >> m$, however optimizing the forward mode implementation could enable users to access fast differentiation for mappings which are of the form $f(x) : R^n \rightarrow R^m$ when $m >> n$.
- Finally, we would like to increase our testing suite. Currently, our testing suite only tests scalar inputs. However, we have already included functionality in our library to allow for both vector input and vector output. Hence, we would like to expand our testing suite to test these cases thoroughly.

2. How will your software change?

- After adding support for additional elementary functions and operations, our software will change in two key ways. First off, the *val_derv.py* file will contain additional instance methods pertaining to the new functions and operations we implement. Specifically, we will have as many new instance methods as additional elementary functions/operations we provide. Additionally, the testing suite file *test_val_derv.py* will contain additional test cases that perform unit testing on these new elementary functions and operations.
- To implement the reverse mode capability, we will need to create a new module, called *reverse_mode.py*. This module will contain the class definition for the reverse mode automatic differentiation and will be set-up similarly to the *forward_mode.py* module. We note that a key implementation detail in the reverse mode will be the underlying data structure we use to represent the computational graph. After a lot of research, we realize that we need a data structure such as a dictionary. This will enable us to save time in retrieving stored operations as the complexity of our outputs increases. In addition to creating the new reverse mode module, we will need to add a new testing file which includes unit and integration tests for reverse mode.
- If we were to optimize our forward mode implementation, we would have to change the underlying data structure which represents the computational graph. A Chain Map data structure would be used instead of our current implementation in order to decrease the number of repetitive calculations and increase efficiency as the input complexity increases.

3. What will be the primary challenges to implementing these new features?

- The primary challenge we will face with implementing additional elementary functions and operations is dealing with the dual number cases for these additions. We have found that many of the elementary functions and operations are simple to implement in the real number case, however when dealing with dual numbers they can become quite complex and so special care must be taken in handling these cases.
- The primary challenge in implementing reverse mode will be understanding the structural and methodological differences between forward and reverse mode. For example, before we can implement the reverse mode module, we need to understand if we can even make use of our code from forward mode as a starting point or if we will have to completely reimplement the reverse mode module from scratch.
- The primary challenge we expect to face with optimizing our forward mode implementation is in the use of a Chain Map data structure. We will have to understand, in detail, how this complex data structure works and look into how our current code implementation would work with such a data structure.

Feedback From Milestone 1

2/2 Introduction: Would have been nice to see more about why do we care about derivatives anyways and why is undefined a solution compared to other approaches?

Response: In the Introduction, we addressed these comments by explaining the purpose of derivatives, expanding upon the real-world applications of derivatives, and their generalizability across multiple dimensions. We addressed this comment in the updated first bullet point of the introduction section.

2/2 Background: Good start to the background. Going forward, I would like to see more discussion on automatic differentiation. How do forward mode and reverse mode work? I would also like to see more discussion on what forward mode actually computes (Jacobian-vector product), the "seed" vector, and the efficiency of forward mode.

Response: In the Background, we addressed these comments by adding four new subsections which discuss the topics of reverse mode, jacobian-vector product, seed vectors, and the efficiency of forward mode. This new information is contained in Part 2, Part 3, Part 7, and Part 8, in the background section.

3/3 How to use: Good Job!

Response: N/A

2/2 Software Organization: Nicely Done!

Response: N/A

4/4 Implementation: Classes and methods are very well thought-through. It would be great if you could list all the elementary operations that you will overload.

Response: In the Implementation, we addressed this comment by listing all fourteen elementary operations which we plan on overloading. We addressed this comment in the subsection "3a. Dual Numbers" under the second bullet point.

2/2 License: Good Job!

Response: N/A