CS207 Final Project: Milestone 2 - November 19 2019

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1 Introduction

Derivatives come up in every aspect of science and engineering. Calculus taught us how to derive analytical expressions of functional derivatives, but in many cases this is either impossible or too much of a hassle. Therefore, numerical methods or algorithmic approaches to compute the derivative are extremely important. Methods of computing functions' derivatives in computer programs can be classified into 4 types:

(1) Determining derivatives by hands and coding them.
(2) Symbolic differentiation in computer tools, such as Mathematica and Maple.
(3) Numerical methods: using finite differences to approximate derivatives.
(4) Automatic Differentiation, which is the subject of our project.

Automatic differentiation (AD) is a set of techniques for evaluating functional derivatives efficiently and accurately in computer programs. For any analytic function f(x) to be differentiated at a point x_0, AD first rewrites f(x) as a combination of elementary functions, then determining the derivative values of f(x) through combining derivatives of elementary functions by the chain rule. Since the derivative values of all elementary functions are known and accurate, and the procedures of AD have no potential sources of errors except tiny rounding errors due to machine precision, thus the derivative values obtained by AD are accurate. As for other differentiation methods, manual calculating functional derivatives and coding them by hands can be tedious, time-consuming and prone to make mistakes; symbolic differentiation could return rigmarole and unreadable symbolic expressions; and numerical method of finite differences could be ill-conditioned due to truncation and round-off errors, and is also inappropriate to handle functional derivatives with many independent variables.

For example, in the numerical method of finite difference, the derivative is calculated as the following where the limit for h is approached but not put to zero:

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h}$$

While this approach yields decent results in many cases, it is never completely accurate. For too large values of h, the error originates from the intrinsic error of the finite difference derivative. For too small values of h, the error originates from rounding errors.

Although AD does not show explicit derivative expressions, people usually only want to obtain derivative values at some points rather than symbolic expressions, thus AD is much better than other differentiation methods with respect to determining functional derivative values.

In modern differentiation computation, AD is the most efficient and accurate tool to implement differentiation in computer programs. In this project, we will design an accurate, user-oriented differentiation calculator by implementing AD.

2 Background

Automatic differentiation is an algorithmic approach to compute derivatives up until machine precision accuracy. It has two common methods: forward and reverse mode. In this project, only the forward mode will be discussed at first. Forward automatic differentiation leverages the chain rule to split the differentiation of a complex function in elementary functions and makes use of the easy derivatives of elementary functions. If $h(u(t))$ is the function of which the derivative is required, the chain rule for partial derivatives says:

$$\frac{\partial h}{\partial t} = \frac{\partial h}{\partial u} * \frac{\partial u}{\partial t}$$

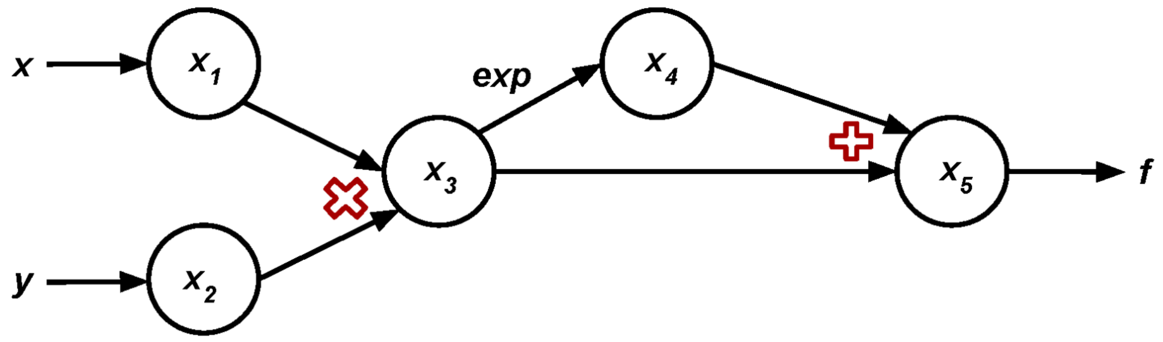
Or for $h(u(t), v(t))$:

$$\frac{\partial h}{\partial t} = \frac{\partial h}{\partial u} * \frac{\partial u}{\partial t} + \frac{\partial h}{\partial v} * \frac{\partial v}{\partial t}$$

Hence, the computation of the derivatives of complicated functions that consist of multiple, consequent elementary operations can be split into the multiplication and addition of derivatives of the elementary functions in the following table. Examples of the elementary operations are addition and multiplication but also sine, cosine and log. The complete list of elementary functions that will be incorporated in this package can be found in 'Implementation'. A subset is illustrated in the table below:

Elementary function	Example
Field Operations	$+ - */$
Powers	x^2, x^6
Roots	$\sqrt{x}$
Trigonometric	$sin(x)$
Inverse Trigonometric	$asin(x)$
Logarithmic	$log(x)$
Exponential	e^x

The split of the complex function into its elementary operations is commonly visualized in a so-called computational graph. This summarizes the sequence of operations that need to be done for the evaluation and differentiation of the function. An example for the simple function $f(x, y) = xy + exp(xy)$ is given in the image below. Note that this example comes from Lecture 12.



The actual implementation of the forward mode can be better understood using the so-called seed vectors p_i for every variable x_i. This means that, every time the derivative of a function is computed, the derivative is 'seeded', or multiplied (dot product) by the corresponding seed. An example might clarify this. Imagine function $f = x * cos(y)$, where x and y are the variables corresponding to seed vectors $p_1 = [1, 0]$ and $p_2 = [0, 1]$ respectively. The directional derivative D_p of f will then be computed as follows:

$$D_p x_3 = \sum_i^n \frac{\partial x_3}{x_i} p_i$$

Where x_1, x_2 and x_3 correspond to x, y and $x * cos(y)$. We can then specify the direction p to find the desired derivative. For instance, for $p = [1, 0]$, we recover:

$$D_p x_3 = \frac{\partial x_3}{\partial x_1} p_1 + \frac{\partial x_3}{\partial x_2} p_2 = \frac{\partial x_3}{\partial x_1} = \frac{\partial f}{\partial x}$$

Or mathematically:

$$D_p x_3 = \nabla x_3 \cdot p$$

This means that the forward mode of automatic differentiation is actually computing the dot product of the gradient and the seed vector. Choosing the seed vectors appropriately, either this product or the full gradient can be recovered, dependent on the application.

For functions in higher dimensions h(x): $\mathbb{R}^m \to \mathbb{R}^n$, the entire Jacobian will be computed using the same, simple approach. Recall the definition of the Jacobian J in $\mathbb{R}^{nxm}$ for function h(x):

$$\mathbf{J} = \begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & .. & \frac{\partial h_1}{\partial x_m} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & .. & \frac{\partial h_2}{\partial x_m} \\ .. & .. & .. & .. \\ \frac{\partial h_n}{\partial x_1} & \frac{\partial h_n}{\partial x_2} & .. & \frac{\partial h_n}{\partial x_m} \end{bmatrix}$$

Note that the seed vector approach is still valid for this high-dimensional case. So teh forward mode is actually computing the product of the Jacobian with the seed vector. Again, the entire Jacobian can be recoverd by choosing the seed vectors appropriately and adding the resulting products.

3 How to Use AutoDiff

3.1 How to install AutoDiff

There are two methods of installing our package: Github and PyPI. The installation details are listed below. After installation, the user should import the class Var, which represents variables, from our package (shown as the pseudocode below) and other dependencies (such as numpy and math) since we import those dependencies to our package modules. With the imported package, the user can define x as an object of Var, and give the initial input of x. Then the user can apply function f on x, which returns f(x) with new values and jacobian.

3.1.1 Installation from Github

- Step 1: Download our package from Github to users' local directory by the following commands in the terminal

  ```
  mkdir AutoDiff
  cd AutoDiff
  git clone https://github.com/BackPropagators/cs207-FinalProject.git
  cd cs207-FinalProject
  ```

- Step 2: Create and Activate a virtual environment in conda.
  - If the user don't have conda, she/he should install it. Then the user can create his/her own virtual environment in conda by the following codes, where yourname is the name the user wants to call the newly created environment.

    ```
    conda create -n yourname python=3.6 anaconda
    ```

  - Activate the user's virtual environment

    ```
    source activate yourname
    ```

  - Install the required dependencies and run the given tests in AutoDiff

    ```
    pip install -r requirements.txt
    pytest
    ```

    If pytest is not installed, then the user can install it by

    ```
    pytest install -U pytest
    ```

  - Use AutoDiff Python package in the terminal (See demo in 3.2)

```
>>> from AutoDiff.ForwardAD import Var
>>> x = Var(1)
>>> f = x + 1
>>> f.get_value()
2
>>> f.get_der()
[1]
...
>>> quit()

# deactivate virtual environment
conda deactivate
```

3.1.2 Installation from PyPI.

We use PyPI to distribute our package in our development of the package.

3.2 Basic Demo

Install our package, and import the module and dependencies

```
pip install AutoDifferentiate
python
>>> from AutoDiff.ForwardAD import Var
>>> import numpy as np
```

instantiate a `Var` class.

```
>>> x = Var(1.0)
```

Define a function.

```
>>> f = x + 1
```

Evaluate the function value which is expected to be 2.0.

```
>>> f.get_value()
2.0
```

Evaluate the function jacobian which is exepcted to be [1.0].

```
>>> f.get_der()
[1.0]
```

Evaluate the value and jacobian of scaler function with one variable.

```
# basic operation
# Expect the value of f is 3.0, and the derivative of f is [2.0]
>>> x = Var(1)
>>> f = 2*x + 1
>>> f.get_value()
3.0
>>> f.get_der()
[2.0]

# exponential function
# Expect the value of f is around 2.718281828459, and the derivative is
 around [2.718281828459]
>>> f = Var.exp(x)
>>> f.get_value()
2.718281828459045
>>> f.get_der()
[2.718281828459045]

# logarithmic function
# Expect the value of f is 0.0, and the derivative of f is around [0.434
29448190325]
>>> f = Var.log(x, b=10)
>>> f.get_value()
0.0
>>> f.get_der()
[0.43429448190325176]

# trignometric function
# Expect the value of f is 0.49999999999999994, and the derivative is
 [0.8660254037844]
>>> y = Var(np.pi/6)
>>> f = Var.sin(y)
>>> f.get_value()
0.49999999999999994
>>> f.get_der()
[0.8660254037844387]
```

4 Software Organization

4.1 Project Directory Structure

```
CS207-FinalProject/
                    README.md
                    LICENSE
                    setup.py
                    requirements.txt
                    AutoDiff/
                             _init_.py
                             ForwardAD.py
                    docs/
                              milestone1.ipynb
                              milestone2.ipynb
                    test/
                         test_all.py
                    demo/
                         presentation.pdf
                    ...
```

4.2 Included Modules and Basic Functionality

AutoDiff: This module includes implementation for classes AutoDiff and Multifunc. AutoDiff and Multifunc implement the forward mode of auto differentiation. AutoDiff takes care of scalar function inputs (with single and multiple variables) and Multifunction takes care of vector function inputs.

Test: This module includes all the test suites for the package.

4.3 Test

The test suites live in *CS207-FinalProject/Test/* folder. We will use Travis CI to run tests and use CodeCov to automatically checks code coverage.

4.4 Distributing Our Package

We will use PyPI to distribute our package. The Python Package Index (PyPI) is a repository of software for the Python programming language.

4.5 Packaging

We will follow the Python Packaging User Guide published by the Python Packaging Authority(PyPA), which is the authoritative resource on how to package, publish, and install Python projects using current tools. We will use Setuptools because it is comprehensive, actively-maintained, and stable to create an package for easy distibution out of our project.

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5 Implementation

5.1 Core Data Structures\ The core data structure for storing the jacobian is python dictionary, where the key is the variable (an instance of `Var` , see **Core Classes** below) and the value is its partial derivative.

5.2 Core Classes\ In the `ForwardAD.py` , we implemented the `Var` class, which defines the variables in a function and calculates the jacobian of scalar function with single and multiple variables (multivariables will be tested in the future; see 5.6 for details). We have also implemented the `MultiFunc` class, which calculates the jacobian of vector functions with single and multiple variables (`MultiFunc` will be tested in the future, so it is not included in the code; see 5.6 for details).

5.3 Important Attributes\ The `Var` class has two private attributes: `self._val` and `self._der` . `self._val` stores the value of the current function, and `self._der` is a dictionary whose key is a `Var` instance and value is its partial derivative. `self._der` is initialized as {self: 1} in the constructor. When there is only one variable in the function, after each operation, only the value (jacobian) may be updated whereas the key (variable) remains the same in the new dictionary. When there are multiple variables in the function, after each operation, values (jacobian) may be updated and new key (variable) may be added in the new dictionary.

5.4 External Dependencies\

- Numpy: We will rely on the `math` and `NumPy` package.

5.5 Elementary Functions\ We defined methods that deal with these elementary functions inside the `Var` class. To use these functions, simply call `Var.function_name` . See demo in 3.2.

5.6 Multivariable Function and Vector Functions\ To get the jacobian of a multivariable function, we ask to user to supply the order of `Var` in a list. The following code demoes the process.

```
from AutoDiff.ForwardAD import Var
>>> x = Var(1)
>>> y = Var(2)
>>> f = x + 2*y
>>> f.get_der([x, y])
[1.0, 2.0]
```

For vector functions, we ask to user to supply the functions in a list. The following code demoes the process.

```
from AutoDiff.ForwardAD import MultiFunc
>>> x = Var(1)
>>> F = MultiFunc([x+1, 2*x])
>>> F.get_der()
[[1], [2]]
```

6 Additional Features

With the forward mode of automatic differentiation up and running, additional features that rely on differentiation up until machine precision can be developed. This section will discuss the mathematical background of the numerical implementation of root-finding and optimization, which will be implemented as additional features of the packages for the final version.

6.1 Root-finding

First, root-finding arises in many applications in any kind of engineering and science. Consider the general problem in which the purpose is to find that x-value that satisfies the following equation for a certain function f:

$$f(x) = 0$$

There are multiple numerical approaches to iteratively find this x-value, including the famous Newton's method. Here, a certain starting value $x^{(0)}$ is chosen, after which the following equation is used to update $x^{(k)}$ until a particular convergence criterium is reached:

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

Note that the derivative of f with respect to x evaluated at $x^{(k)}$ plays a crucial role in this equation. In many cases, analytical expressions for $f'(x)$ are not available and numerical differentiation methods are needed. With the forward mode of the automatic differentiation working, the Newton's method for root-finding can be implemented. The use can interact as follows with this module of the package AutoDiff:

```
>>> from AutoDiff.ForwardAd import Var
>>> from AutoDiff.root_finding import Newton
>>> f = lambda x: x**2-1
>>> guess = 2
>>> root = Newton(f, guess)
1.0
```

The iterated roots in the above algorithm can be illustrated by the plot below.

6.2 Optimization

A second, highly relevant application of numerical differentiation can be in optimization. In many problems, and most notably in Computer Science and Machine Learning in the last years, is it crucial to efficiently minimize a certain function F in terms of multiple variables $\mathbf{x} = (x_1, \ldots, x_n)$. Or mathematically:

$$\mathbf{x}_{solution} = \underset{\mathbf{x}}{argmin} F(\mathbf{x})$$

Inside the same function called 'optimize', two numerically distinct methods will be incorporated to find the value of the funtion's parameters that correspond to a minimum: gradient descent and BFGS.

6.2.1 Gradient Descent

Firstly, a very common numerical method that iteratively computes the solution for this equation is gradient descent. In this algorithm, an initial guess is iteratively updated by the taking a step in the direction that is alligned with the steepest descent - or in the opposite direction of the gradient at that particular value. This leads to the following equation:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \gamma \nabla F(\mathbf{x}^{(k)})$$

Here, γ is called the 'learning rate' and corresponds to the size of the step taken in the steepest direction. Again, it is crucial to accurately compute the gradient $\nabla F(\mathbf{x}^{(k)})$ in every iteration and this is where the automatic differentiation package comes in. The user is able to use the optimization function as follows:

```
>>> from AutoDiff.ForwardAd import Var
>>> from AutoDiff.optimize import optimize
>>> def f(vars):
      x,y = vars
      return (x-1)**2 - Var.sin(y)**4
>>> guess = [0.1, 0, 2]
>>> gamma = 0.1
>>> argmin, min_F, n_iter, norm_der = optimize(F, guess, solver = 'GD',
                                   tolerance=10e-8, max_iter=200, gd_lr=gamma)
```

There are a couple of important function input parameters and output variables to clarify here. For solver a string 'GD' is given as input, corresponding to the gradient descent. The tolerance defines the convergence criterium of the method; the gradient descent method stops after the norm of the gradient at the current iteration point is smaller or equal to the specified floating point number. The user can also specify max_iter, the maximum number of iterations the algortithm executes. This is the stopping criterium whenever the convergence criterium has not been met. The gd_lr simply corresponds to the learning rate used in the method.

Note that argmin stands for the array of values for $\mathbf{x}$ that minimizes F, min_F corresponds of the actual value of the function F at that minimum and n_iter equals the number of iterations executed. This number can either be equal to n_iter or smaller than max_iter when the convergence criterium has been met at a previous iteration. Lastly, norm_der is equal to the norm of the derivative in the last iteration point.

Also, it can be useful for the user to have some practical knowledge about the behaviour of gradient descent. For instance, the gradient descent algorithm does not guarantee an absolute minimum and that for complicated functions it is common to end up in a local minimum - since the gradient is also equal to zero at this point. Note that for many applications, these local minimima can satisfy the requirements. Also, whenever the method appears to diverge, the user might want to decrease the learning rate.

6.2.2 The Broyden Fletcher Goldfarb Shanno method (BFGS)

A second, more sophisticated and faster numerical method that is incorporated in the optimize function is the Broyden Fletcher Goldfarb Shanno method, or simply 'BFGS'. In order to understand its use, it is useful to first discuss the widely know Newton optimization method. Here the initial guess is iteratively updated as follows:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - [\mathbf{H}(\mathbf{x}^{(k)})]^{-1}\nabla f(\mathbf{x}^{(k)})$$

Here $\mathbf{H}$ corresponds to the Hessian matrix evaluated at $x^{(k)}$. This method is widely known due its quadratic convergence, but in practice it is either very hard or computationally costly to compute the Hessian. This is why the Newton has not been implemented in this package.

However, the BFGS method serves as a trade-off in convergence and computational cost. Every iteration, the following expressions are executed:

- Solve $B^{(k)} s^{(k)} = -\nabla f(x^{(k)})$ for step $s^{(k)}$
- $x^{(k+1)} = x^{(k)} + s^{(k)}$
- $y^{(k)} = \nabla f(x^{(k+1)}) - \nabla f(x^{(k)})$
- $\Delta B^{(k)} = \frac{y^{(k)}(y^{(k)})^T}{(y^{(k)})^T s^{(k)}} - \frac{B^{(k)} s^{(k)} (s^{(k)})^T B^{(k)}}{(s^{(k)})^T B s^{(k)}}$
- $B^{(k+1)} = B^{(k)} + \Delta B^{(k)}$

With the identity matrix as initial guess for B, the iterative update on B makes the matrix accumulate second-order derivative information and therefore approach the Hessian. This means that, after some iterations, the method will start behaving like Newton's method and thus converge quadratically without having to compute the Hessian. Recognizing this numerical advantage, the BFGS method has been incorporated in the package. The user is able to use it as follows:

```
>>> from AutoDiff.ForwardAD import Var
>>> from AutoDiff.optimize import optimize
>>> def f(vars):
      x,y = vars
      return (x-1)**2 - Var.sin(y)**4
>>> guess = [0.1, 0, 2]
>>> argmin, min_F, n_iter, norm_der = optimize(f, guess, solver = 'BFGS'
,
                              tolerance=10e-8, max_iter=200)
```

Here, everything is similar to the optimize code as described above except for the specification of 'BFGS' as solver and the absence of a learning rate.

Note that, thanks to its superlinear convergence, the user will experience faster convergence than the gradient descent method, so lower n_iter.

7 Future Extensions

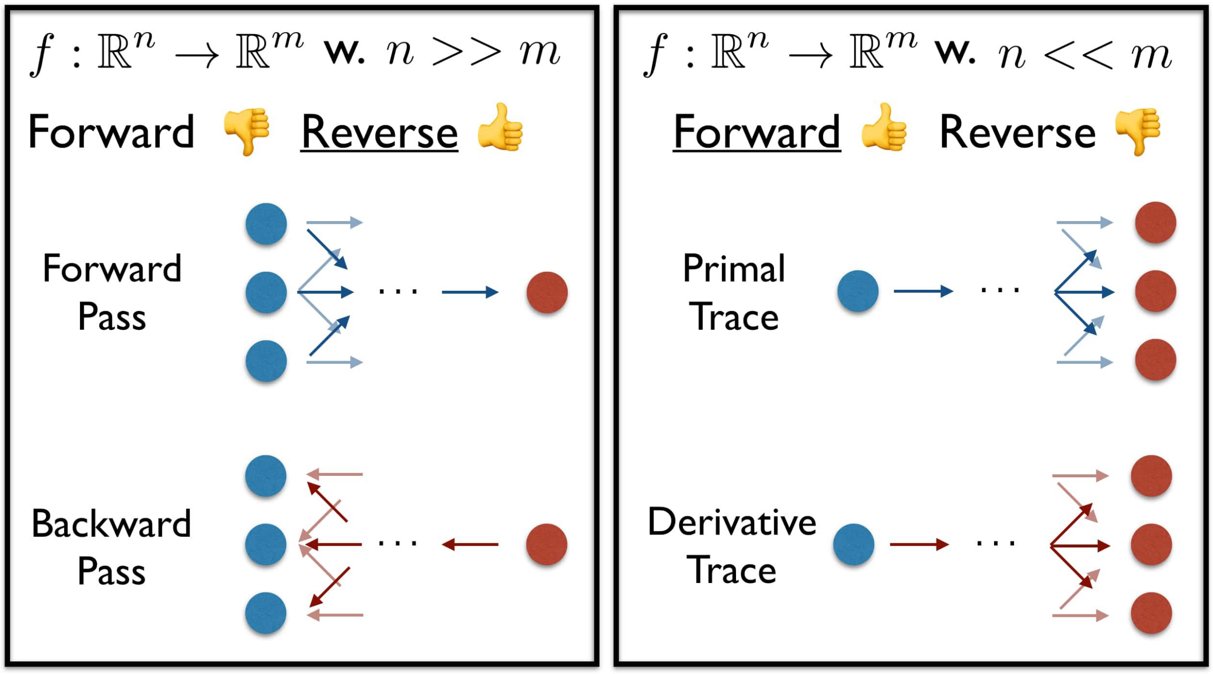
For future extensions of the package, we consider the following:

7.1 Reverse Mode

The AutoDiff Package implements the forward mode AD. We can also implement AD using reverse mode. While forward and reverse modes give the same answer, there are some differences between them:

1. Forward mode calculation depends on number of independent variables while the reverse mode calculation does not depend on the number of independent variables.
2. As for memory storage, Forward mode requires us to store the derivatives, while reverse mode AD only requires storage of the activations.
3. As for the time of computation, Forward mode AD computes the derivative at the same time as the variable evaluation while the reverse mode does so in the separate backward phase.

Considering the differences, when the number of functions to evaluate is much greater than the number of inputs (n << m), forward mode is more efficient. When the number of inputs is much greater than the number of functions (n >> m), reverse is more efficient. We would want to implement the reverse mode AD and allow user to choose between these two modes.


$f : \mathbb{R}^n \to \mathbb{R}^m$ w. $n >> m$
Forward 👎 Reverse 👍
Forward Pass
Backward Pass
$f : \mathbb{R}^n \to \mathbb{R}^m$ w. $n << m$
Forward 👍 Reverse 👎
Primal Trace
Derivative Trace

7.2 Higher Order Derivatives & Mixed Derivatives

Another extension we could add to our package is to make it capable of calculating higher order derivative and mixed derivatives. Then we could further implement 2nd order optimization algorithms like the Hessian matrix optimization.

7.3 More Root Finding Algorithms

The AutoDiff package implements the Newton Method for root finding. Newton method is fast but does not guarantee convergence. One root finder method that guarantees convergence is the Bisection method. The idea of Bisection is to trap a root in a shrinking interval. This method is slow but dependable.

Secant method is another root finder algorithm we could add to our package. This method does not require derivative and is also fast.It uses a succession of roots of secant lines to better approximate a root of a function f. The secant method can be thought of as a finite-difference approximation of Newton's method.

8 Conclusion

The AutoDiff package offers easy-to-use, computationally efficient differentiation with machine precision accuracy:

1. Implements the forward mode of automatic differentiation
2. Straight-forward to install through PyPI or Github
3. Offers built-in root-finding and optimization algorithms
4. Future extensions include reverse mode, higher order derivatives and a broader spectrum of root-finding methods

In [0]:

```
```

In [0]:

```
```