A Python Package for Automatic Solution of Ordinary Differential Equations with Spectral Methods

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Abstract—We present a Python module named PyCheb, to solve the ordinary differential equations by using spectral collocation method. PyCheb incorporates discretization using Chebyshev points, barycentric interpolation and iterate methods. With this Python module, users can initialize the ODESolver class by passing attributes, including the both sides of a given differential equation, boundary conditions, and the number of Chebyshev points, which can also be generated automatically by the ideal precision, to the constructor of ODESolver class. Then, the instance of the ODESolver class can be used to automatically determine the resolution of the differential equation as well as generate the graph of the high-precision approximate solution.

Keywords—numerical methods, spectral collocation method, Python, ODEs.

I. INTRODUCTION

Differential equations are used to describe phenomena of states and processes. Solutions of these problems explain patterns of them, thus people are eagerly to seek solutions of these equations for describing states and making predictions of the future. An ordinary differential equation is a differential equation containing one function (as the variable of the equation) of one independent variable (of the function) and its derivatives. Solving ODE is comparatively easy but useful for scientists and engineers. Therefore, in this paper, we investigate how to solve ODE numerically only.

Spectral methods are a class of numerical techniques used in applied mathematics to solve differential equations numerically. The idea is to write the solution of the differential equation as a sum of certain "base function" (for example, as a Fourier series which is a sum of sinusoids) and then to choose the coefficients in the sum in order to satisfy the differential equation at any given accuracy [1]. Spectral methods can be used to solve ordinary differential equations (ODEs), partial differential equations (PDEs) and eigenvalue problems involving differential equations. In this paper, we use the spectral collocation method.

An object-oriented MATLAB system named Chebfun was created by a group of developers leading by Prof. Trefethen in the University of Oxford in 2002. This system allows users to naturally input the ordinary differential equations in MATLAB code and get the solutions by using spectral methods. Our project PyCheb is inspired by Chebfun. The reason why we implement spectral collocation method in Python is that first, Python is a high-level programming language and has a maturing ecosystem of scientific libraries, so it powerful enough for the implementation of this ordinary differential equation solving algorithm. Besides, Python is a general-purpose language, so it is not only used in academic settings but also in industry. Therefore, compared to the MATLAB implementation, it can be more widely used, by both scientists and engineers. Also, it is more convenient and easily to use. Furthermore, we expect to accelerate our system in the future by taking the advantages of GPU computing. This is important as we plan to expand our algorithm to solving partial differential equations, which is more complicated in computing. Python modules like PyCUDA and Theano can help us achieve our goal. Thus, the Python implementation has a high extensibility.

Our Python module described in this paper can automatically solve the ordinary differential equations using spectral collocation method and plot the graph of the high-precision approximate solution. In order to solve an ordinary differential equation, users need to initialize a instance of the ODESolver class, and pass attributes including the left hand side and right hand side of the object equation, the boundary conditions and boundary values, and the number of Chebyshev points, to the constructor of Polyfun class, in particular, we can set a precision and let the algorithm to choose enough points to do the calculation. Then, by calling the solve() method, users can get the solutions step by step automatically. The detailed process will be elaborated in the following sections.

II. FEATURES AND BASIC USAGE

In this section, the process of solving ordinary differential equations (ODE) is described step by step.

The users first need to initialize an instance of the ODESolver class. ODESolver is a class for the ordinary differential equations solver. The constructor of the class is defined as follow:

```python
def __init__(self, lfunc, rfunc, domain, lvalue, rvalue, N = 10)
```

lfunc means the left hand side of the ODE, and rfunc means the right hand side of the ODE. domain refers to the boundary of the ODE. lvalue is the left boundary value and rvalue is the

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1 http://www.chebfun.org.
2 https://mathema.tician.de/software/pycuda/
3 http://deeplearning.net/software/theano/
4 In general cases the accuracy can be set by users themselves
right boundary value. \(N\) represents the number of Chebyshev points.

For example, we want to solve the ODE:

\[ u'' = e^{2x}, -1 < x < 1, u(\pm1) = 0 \]

We can initialize an Polyfun instance like:

```python
ger = import PyCheb
ger = PyCheb.Polyfun("diff(u,2)", \"math.exp(2*x)\", [-1,1], 0, 0, 16)
```

Having these parameters, the instance of Polyfun class can start to solve the ODE using 16 Chebyshev points on the interval \([-1,1]\).

### A. Chebyshev Points [7]

**Definition II.1.** Suppose \(\{z_j\}\) are \(n+1\) equidistant points on the upper half of the unit circle in the complex plane. The Chebyshev points associated with the parameter \(n\) are the real parts of these points,

\[ x_j = \Re z_j \quad 0 \leq j \leq n \quad (1) \]

**Definition II.2.** Chebyshev points is in terms of the original angles:

\[ x_j = \cos\left(\frac{j}{n}\right) \quad 0 \leq j \leq n \quad (2) \]

In our Python module, the Chebyshev points is generated by calling the `getChebPoints()` function:

```python
>> f.getChebPoints()
```

The return value of `getChebPoints()` is a list of Chebyshev points:

### B. Spectral Accuracy

The reason why we choose spectral collocation method to solve ODE is that this method is naturally with an advantage of super-fast convergence rate when the object function is smooth. Thus users can get a high-precision solution of an ODE problem at a low computing cost [2].

The following MATLAB programs compare the finite difference approximation \(w_j\) with the exact derivative, \(-e^{\cos(x)}\sin(x)\), for various values of \(N\).

The first MATLAB program uses the traditional finite difference process:

```matlab
Nvec = 2^(3:12);
clf, subplot('position', [.1 .4 .8 .5])
for N = Nvec
    h = 2*pi/N;
    x = -pi + (1:N)*'h';
    u = exp(cos(x)); uprime = -sin(x).*u;
    e = ones(N,1);
    D = sparse(1:N, [2:N 1], 2*e/3, N,N) -
        sparse(1:N, [3:N 1 2], e/12, N,N);
    D = (D-D')/h;
    error = norm(D*u-uprime, inf);
    loglog(N, error, '.', 'markersize', 15), hold on
end
grid on, xlabel N, ylabel error
title('Convergence of 4th-order finite difference')
semilogy(Nvec, Nvec.^(-4), '--')
text(105,5e-8,'N^{-4}', 'fontsize', 18)
```

Fig. 1. Convergence result using finite different differentiation

The second MATLAB program uses spectral method. From the output graph we can see that the errors decrease very rapidly until such high precision is achieved that rounding errors on the computer prevent any further improvement:

```matlab
for N = 2:2:100;
    h = 2*pi/N;
    x = -pi + (1:N)*'h';
    u = exp(cos(x)); uprime = -sin(x).*u;
    column = [0 .5*(-1).^(1:N-1).*cot((1:N-1)*h/2)];
    D = toeplitz(column, column([1 N:-1:2]));
    error = norm(D*u-uprime, inf);
    loglog(N, error, '.', 'markersize', 15), hold on
end
grid on, xlabel N, ylabel error
title('Convergence of spectral differentiation')
```

Fig. 2. Convergence result using spectral method
This phenomena is called spectral accuracy. As $N$ increases, the error in a finite difference or finite element scheme typically decreases like $O(N^{-m})$ for some constant $m$ that depends on the order of approximation and the smoothness of the solution. For a spectral expansion, convergence at the rate $O(N^{-m})$ for every $m$ is achieved, provided the solution is infinitely differentiable, and even faster convergence at a rate $O(c^N)(0 < c < 1)$ is achieved if the solution is suitably analytic.

C. Chebyshev Differentiation Matrix

A proper discretization is of vital importance in numerical methods for differential equations. For any smooth functions, the discretization of its first order derivative can be written in the form of matrix, namely Chebyshev differential matrix.

Chebyshev differentiation matrix has the following arithmetic expression [2]:

\[(D_N)_{ij} = \frac{c_i}{c_j} \frac{(-1)^{i+j}}{(x_i - x_j)^2}, i \neq j, i, j = 1, ..., N - 1\]

Where

\[c_i = \begin{cases} 2, & i = 1orN, \\ 1, & otherwise \end{cases}\]  

(3)

In PyCheb, we can obtain the Chebyshev differentiation matrix $D_N$ by:

```python
>> f = PyCheb.Polyfun("diff(u,2)", "math.exp(2*x)", [-1,1], 0, 0, 16)
>> f.getChebMatrix()
```

Chebyshev differentiation matrix is important in solving ODEs with the spectral method, we need to use it to solve the boundary value problems arising in ordinary differential equations.

As our first example, the ODE:

```python
>> import PyCheb
>> f = PyCheb.Polyfun("diff(u,2)", "math.exp(2*x)", [-1,1], 0, 0, 16)
>> f.solve(isLinear=1)
```

To obtain the solution of this ODE, sometimes we need compute the second derivative $u''$. In this case, the most practicable way is to consider it as a linear operator [3]. Thus we can compute the second derivative operator in the following form: $D_N^2 = (D_N)^2$. Generally a linear operator is created by replacing the $\text{diff}(u, k)$s (which means the $k$th derivative of $u$) and the linear combination of them, in the left hand side by

\[L(u) = \sum_{i=0}^{i=k} C_i D_N^j(u) \quad C_i \text{ are constant.}\]  

(4)

Another example is for ODE [4]:

\[u'' + u' + 100u = x, -1 < x < 1, u(\pm1) = 0\]

To initialize an instance of ODESolver class for this ODE with Chebyshev points number of 16:

```python
>> import PyCheb
```

In PyCheb, the linear operator for this ODE can be obtained by passing the Chebyshev matrix $D_N$ as parameters into the method `getL()`:

```python
>> D = f.getChebMatrix(N)
>> f.getL(D)
```

D. Solving Linear(general cases) and Nonlinear ODEs

Now we enter the final step of solving an ODE. In this step, ODEs are divided into linear and nonlinear ones. For each type, we use different methods to solve them.

1) Linear ODE: With the linear operator in hand, solving a linear ODE becomes a matter of solving a linear system of equations. We use the following linear ODE as an example:

\[u'' = e^{2x}, -1 < x < 1, u(\pm1) = 0\]

Using PyCheb, we can solve this linear ODE with a given number of points simply by:

```python
>> import PyCheb
>> f = PyCheb.Polyfun("diff(u,2)", "math.exp(2*x)", [-1,1], 0, 0, 16)
>> f.solve(isLinear=1)
```

We can also set an ideal precision first and solve the problem:

```python
>> import PyCheb
>> f = PyCheb.Polyfun("diff(u,2)", "math.exp(2*x)", [-1,1], 0, 0, precision=1e-5)
>> f.solve(isLinear=0)
```

In method `solve()`, Chebyshev points are first calculated and substituted into the right hand side of the ODE. The result is a set of values, we call it `ys`. Then, the Chebyshev matrix and linear operator are calculated. To solve the linear ODE as a linear system of equations, we just need to use the inverse of linear operator to multiply `ys`. In method `solve()` all these steps are automatically processed, and its return value is a set of values for $u$.

2) Nonlinear ODE: Take the following nonlinear ODE as an example:

\[u'' = e^{2u}, -1 < x < 1, u(\pm1) = 0\]

Because of its nonlinearity, it is no longer simply enough to invert the linear operator like the linear ODE example. Instead, the problem must be solved iteratively. An initial guess is chosen first, and here we have the vector of zeros. Then by iterating repeatedly, the system of equations can be solved.

In PyCheb, we only need to solve this nonlinear ODE with a given number of points by:

```python
>> import PyCheb
>> f = PyCheb.Polyfun("diff(u,2)", "math.exp(2*u)", [-1,1], 0, 0, N=16)
```

In normal cases $k \leq 3$.\footnote{In normal cases $k \leq 3$.}
Like the linear cases, we can set the precision first and solve it:

```python
>>> import PyCheb
>>> f = PyCheb.Polyfun("diff(u,2)",
"math.exp(2*u)", [-1,1], 0, 0, precision=1e-4)
>>> f.solve(0)
```

### E. Barycentric Interpolation

Whether by using `solve(isLinear=1)` or `solve(isLinear=0)`, the return value is a set of values for $u$ on Chebyshev points. By using Barycentric interpolation, we can use an unique polynomial to approximate the solution with high precision.

In PyCheb, we can use the `barycentricInterpolate()` function to obtain the high-precision approximate solution expression. Using the linear ODE example:

```python
>>> import PyCheb
>>> f = PyCheb.Polyfun("diff(u,2)",
"math.exp(2*x)", [-1,1], 0, 0,N=16)
>>> xs = f.getChebPoints()
>>> us = f.solve(isLinear=1)
>>> poly = f.barycentricInterpolate(xs, us)
```

`poly` is a vector of coefficients of the polynomial for the high-precision approximate solution.

### F. Plotting

In PyCheb, we can plot the high-precision approximate solution for an ODE by using the `plot()` method. A vector of coefficients of the polynomial for the high-precision approximate solution needs to be passed to `plot()`. For example, for the previous linear ODE:

```python
>>> import pycheb
>>> ...
>>> poly = f.barycentricInterpolate(xs, us)
>>> f.plot(poly)
```

In the example of linear case, we can draw the solution with the following code:

```python
>>> f = PyCheb.ODEsolver("diff(u,2)",
"math.exp(x)", [-1,1], 0, 0, precision=1e-11)
>>> f.solve(1)
```

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**III. Conclusion**

PyCheb is a Python package for solving ordinary differential equations. It implements the algorithm of spectral collocation method, which is of high efficiency in solving ordinary differential equations because of its fast convergence rate. PyCheb can automatically obtain the high-precision approximate solution for the ODE and plot the graph. Although it is a partial implementation for now in the whole vision, it is more light-weighted and can be more widely used in both academic settings and industry. However, currently, PyCheb is a preliminary version. It can only solve ODEs. It still needs to get further improved to be more universal. The next step of our team is to make PyCheb can solve all kinds of ODEs and extend to solving partial differential equations(PDEs), which is more useful as well as more complicated. Moreover, we are about to use GPU computing methods to accelerate the speed of our algorithm. The speedup is important especially for solving more complicated PDE problems.

**References**

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