Doctoral Thesis Research Proposal

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Introduction

Literature Review

Differential Equations

In this section, I discuss elements of differential equation theory. I begin by delineating between different types of differential equations. I then discuss sufficient conditions for existence and uniqueness of solutions to differential equations, followed by a discussion of computing analytic representations of said solutions. I conclude this section with numerical methods for solving differential equations.

What is a Differential Equation

For the purposes of this proposal, a differential equation is an equation relating an unknown function of a single variable to it's derivative. In general, I will be concerned of differential equations of the form

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(t, \mathbf{y}(t); \boldsymbol{\theta}) \tag{1}$$

Here, $\mathbf{F} : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is a vector field, and $\boldsymbol{\theta} \in \mathbb{R}^m$ is a vector of parameters for the differential equation. From here forth, we supress the dependency on $\boldsymbol{\theta}$, but understand that $\mathbf{F}$ may depend on unknown parameters. Differential equations of these forms are called *ordinary differential equations* (ODEs) since they are deterministic and involve derivatives of a single variable. Often, equation (1) is accompanied by a value of $\mathbf{y}$ evaluated at a point in it's domain. This is called an *initial condition* and is written as $\mathbf{y}(t_0) = \mathbf{y_0}$ for some $t_0 \in \mathbb{R}$. The conjunction of equation (1) and an initial value is referred to as an *initial value problem.*

Various complications to equation (1) yield different types of differential equations. If the equation involves partial or mixed partial derivatives, it is called a *partial differential equation.* If $\mathbf{F}$ is a function of a past state of $\mathbf{y}$, it is called a *delay differential equation.* If one, or more, components of $\mathbf{F}$ is a stochastic process, it is called a *stochastic differential equation.* I will not be concerned with these differential equations in this proposal.

Existence & Uniqueness

Not every differential equation which can be written down has a solution. There are sufficient conditions on $\mathbf{F}$ which guarantee a unique solution exists in a bounded region. I present those conditions here without formal proof.

Consider a differential equation described by equation (1) with the initial condition $\mathbf{y}(t_0) = \mathbf{y_0}$. So long as $\mathbf{F}$ is continuously differentiable in a neighbourhood of $(t_0, \mathbf{y_0}) \in \mathbb{R} \times \mathbb{R}^n$, then there is a neighbourhood of the point t_0 such that a unique solution to equation (1) exists satisfying the initial condition.

For the purposes of this proposal, we need only check that $\mathbf{F}$ is continuously differentiable to ensure a solution exists. For a full proof of this theorem, see [1, 2].

Solutions for Ordinary Differential Equations

Not every differential equation which has a solution can have that solution written in terms of algebraic and transcendental functions. In particular, this proposal will be concerned with first order linear differential equations, which do have an analytic representation of their solution. Consider a differential equations of the form

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}(t)\mathbf{y}(t) + \mathbf{g}(t) \,. \tag{2}$$

Here, $\mathbf{A} : \mathbb{R} \to \mathbb{R}^{n \times n}$ which may not necessarily be diagonalizable and $\mathbf{g} : \mathbb{R} \to \mathbb{R}^n$. In general, the solution to equation (2) can be written in terms of fundamental matrices, namely

$$\mathbf{y}(t) = \boldsymbol{\psi}(t)\boldsymbol{\psi}^{-1}(t_0)\mathbf{x}_0 + \boldsymbol{\psi}(t) \int_{t_0}^{t} \boldsymbol{\psi}^{-1}(s)\mathbf{g}(s) \, ds \,, \tag{3}$$

Here, $\boldsymbol{\psi}(t)$ is a fundemantal matrix for equation (2). Our key observation here is that so long as the ODE can be form of equation (2), then the solution can be written in terms of analytic functions. For more on solutions to linear differential equations, see [3].

Numerical Solutions to Ordinary Differential Equations

Not every solution to an ODE which *can* be expressed in terms of analytic functions *should* be expressed in terms of analytic functions. If equation (1) contains many parameters, then equation (3) may be sufficiently complex so that evaluation of $\mathbf{y}(t)$ is not practical. In cases like these, or in cases where the solution can not be found in terms of analytic functions, a rich literature of numerical solutions to differential equations exists.

Consider a scalar form of equation (1)

$$\frac{dy}{dt} = f(t, y) \,, \quad y(t_0) = y_0 \,. \tag{4}$$

By approximating the derivative via a finite difference,

$$\frac{y(t_0 + h) - y(t_0)}{h} \approx f(t_0, y(t_0))$$

$$y(t_0 + h) \approx y(t_0) + h \cdot f(t_0, y(t_0))$$

$$y_{n+1} \equiv y_n + h \cdot f(t_n, y_n) \tag{5}$$

Equation (5) is known as *Euler's Method* [3]. The method successively approximates the true solution at a finite set of times. Euler's method is equivalent to numerical integration of the ODE. From the fundamental theorem of calculus, equation (4) is equivalent to

$$y(t) - y(t_0) = \int_{t_0}^{t} f(s, y(s)) \, ds \,.$$

If we wish to evaluate the solution at $t_0 + h$, we approximate the integral using a Reimann sum

$$y(t_0 + h) = y(t_0) + \int_{t_0}^{t_0+h} f(s, y(s)) \, ds$$
$$\approx y(t_0) + (t_0 + h - t_0) \cdot f(t_0, y(t_0)) \tag{6}$$

In either formulation of Euler's method, h is known as the *step size*. Though in general $y(t_0 + h) \neq y(t_0) + hf(t_0, y(t_0))$, if h is sufficiently small, then the result from Euler's method is an acceptable approximation, assuming that y changes linearly with f as its slope. In principle, in the limit as $h \to 0$, the approximations should can become arbitrarily good[1]. Of course, not all step sizes are practical, which has motivated the study of better numerical methods for approximating the solution to a differential equation.

Quality of a Numerical Solution

Since Euler's method is an approximation, it admits some error between the computed numerical solution and the exact solution. Assessments on the quality of a numerical solution can be examined in terms of the *residual*. For any given ODE, if we knew the analytic solution we would find that $dy/dt - f(t, y(t)) = 0$ identically. Since a numerical methods return approximate solutions on a finite set of points (which can then be interpolated via a desired interpolation scheme) then for an interpolated solution, $z(t)$, it will be the case that $dz/dt - f(t, z(t)) = \Delta(t) \neq 0$ in general $\forall t$. The function $\Delta(t)$ is called the *residual*.

The *order of a method* is defined as $\mathcal{O}(\Delta(t))$ and is usually expressed in terms of the step size h. For instance, Euler's method can be shown to be a $\mathcal{O}(h)$ method [4], which means the residual is proportional to the step size. Smaller steps mean a smaller residual (and thus more accurate solution), but obtaining a desired accuracy may mean taking step sizes too small to be practical.

Most texts on numerical solutions to differential equations use the *local error* as a measure of the quality of a solution. Local error can be interpreted as the error incurred on the nth step when there is no error in the $n - 1^{st}$ step, and is usually expressed as a function of the step size h. Alternatively, the local error is the error between $z(t_1)$ and $y(t_1)$. It can be shown that Euler's method has $\mathcal{O}(h^2)$ local error, assuming f has bounded third derivative [4].

Superior Methods for Numerical Solutions

Euler's method is not usually used in practice for solving differential equations because of it's large local error. Better methods, such as Runge-Kutta Methods, which have $\mathcal{O}(h^5)$ local error [3], which is three orders of magnitude more accurate than Euler's method.

The method involves a weighted average of evaluations of f at various points. The scheme is written as

$$y_{n+1} = y_n + h\left(\frac{k_{n1} + 2k_{n2} + 2k_{n3} + k_{n4}}{6}\right) \tag{7}$$

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[1]though some care should be taken to ensure the solution converges [4].

where

$$k_{n1} = f(t_n, y_n)$$
$$k_{n2} = f(t + 0.5h, y_n + 0.5hk_{n1})$$
$$k_{n3} = f(t + 0.5h, y_n + 0.5hk_{n2})$$
$$k_{n4} = f(t_n + h, y_n + hk_{n3})$$

This method has residual $\mathcal{O}(h^4)$ and local error $\mathcal{O}(h^5)$ [3], which may explain why MATLAB's implementation of this method is titled `ode45`.

Other numerical schemes exist which can improve the accuracy further, adding in adaptive step sizes to control the size of the error [4], or to decrease the local error by another order of magnitude, or to solve what are known as *stiff problems*. Though these complications are interesting, they are not relevant for the purposes of this proposal.

References

[1] Richard K Miller and Anthony N Michel. *Ordinary differential equations*. Academic Press, 1982.

[2] Morris. Tenenbaum and Harry Pollard. *Ordinary differential equations: an elementary textbook for students of mathematics, engineering, and the sciences*. Dover Publications, 1963.

[3] WE Boyce and RC DiPrima. Differential equations elementary and boundary value problems, 2012.

[4] Robert M Corless and Nicolas Fillion. A graduate introduction to numerical methods. *AMC*, 10:12, 2013.