

Math 104A - Intro to Numerical Analysis

NUMERICAL SOLUTION OF ODE

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FALL 2022



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Intro

Before we begin

- Computational HW2 is due Nov 29.
- Some answers to “Would you think of a more intuitive, informal description of Lipschitz function?”
 - ▶ It's very similar to the contraction mapping theorem however the L is not restricted in a closed interval.
 - ▶ I am confused about “C” (ODE was a lil confusing)
 - ▶ y value never goes to plus minus infinity?
 - ▶ function can be partially discontinuous
 - ▶ no i would not come up with something more intuitive. if i dont fully understand it
 - ▶ I think the rate of change of the function cannot exceed the rate of change of the domain, you will get a infinite L in that way. (L looks like a magnifying function that takes the difference between two inputs of f)
 - ▶ bounding slope through outputs
 - ▶ lipschitz function isn't infinitely steep at one point

PROBLEM OF INTEREST

Given $\vec{f} : \mathbb{R}^{1+d} \rightarrow \mathbb{R}^d$, and $\vec{x}_0 \in \mathbb{R}^d$, find $\vec{x} : I \rightarrow \mathbb{R}^d$, where $t_0 \in I \subset \mathbb{R}$ (often $I = [0, T]$) satisfying

$$\dot{\vec{x}}(t) = \vec{f}(t, \vec{x}(t)) \quad (t \in I), \quad \vec{x}(t_0) = \vec{x}_0$$

Example: (Lorenz equation; $d = 3$)

$$\vec{x}(t) = \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} \text{ and } f(t, x, y, z) = \begin{bmatrix} \sigma(y - x) \\ x(\rho - z) - y \\ xy - \beta z \end{bmatrix}$$

If we set $\sigma = 1, \rho = \frac{1}{9}, \beta = 2$.

$$\begin{cases} x_t = y - x, \\ y_t = -xz + \frac{1}{9}x - y, \\ z_t = xy - 2z, \end{cases} \quad \begin{bmatrix} x(0) \\ y(0) \\ z(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad (1)$$

- $(\dot{})$ denotes time derivative $\frac{d}{dt}()$.
- \vec{f} is called the **slope function**.
- The first piece is called ordinary differential equation (**ODE**) while the second **initial condition**, and altogether an initial value problem (**IVP**).
- f is independent of t in this example, but may depend on time in general.

PROBLEM OF INTEREST



Plan

- We mainly focus on one dimensional case ($d = 1$). However, most of the important concepts and intuition are readily extended to higher dimensions (assuming proficiency in vector calculus).

Problem of interest (IVP)

$$\begin{cases} \dot{x} = f(t, x) \\ x(t_0) = x_0 \end{cases}$$

- ODE (more or less synonymous to dynamical system) is a rather general model for physics, biology, etc, anything that depends on time smoothly.
- Since the solution is a function of t (time), it is often called a **trajectory**.

EXISTENCE AND UNIQUENESS OF EXACT SOLUTION

$$\begin{cases} \dot{x} = f(t, x) \\ x(t_0) = x_0 \end{cases} \quad (\text{IVP})$$

Theorem (Existence and uniqueness 1)

If f is continuous on a rectangle centered at (t_0, x_0) , $D = \{(t, x) : |t - t_0| \leq \alpha, |x - x_0| \leq \beta\}$, then (IVP) has a solution on $(t_0 - r, t_0 + r)$, where $r = \min(\alpha, \beta/M)$ and $M = \max_{(t,x) \in D} |f(t, x)|$. If, in addition, $\partial f / \partial x$ is continuous on D , then the solution is unique.

Example

Verify that an IVP $x'(t) = x^{2/3}$ subject to $x(0) = 0$ has a solution around $t = 0$, but it is not unique.

- Are you trying to find something that exists?
- If so, does it stay the same every time you find it?
- We don't prove existence theorem
- Don't get overwhelmed by the theorem, in particular, by its details. Focus on the big picture to begin with.
- In words, "if slope function is nice, the system evolves deterministically at least for a short time."

Theorem (Existence and uniqueness 2)

If f is continuous on $[a, b] \times \mathbb{R}$ satisfies the Lipschitz condition in the second variable, x , i.e., there is $L > 0$ such that for all $t \in [a, b]$,

$$|f(t, x) - f(t, y)| \leq L|x - y|$$

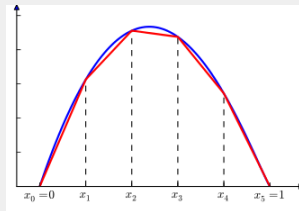
the (IVP) has a unique solution on $[a, b]$.

Remark (Continuous, Lipschitz continuous, continuously differentiable functions of one variable)

Note that the following inclusions, where UC (nonstandard notation) means uniformly continuous functions,

$$C^1[a, b] \subset \text{Lip}[a, b] \subset UC[a, b] = C[a, b].$$

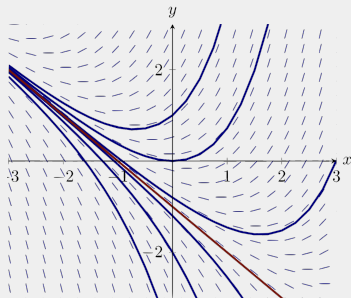
- To make the statement true, we end up needing to classify functions finer and finer.
- **Subjective question:** Lipschitz functions are very important class. Would you come up with a more intuitive, informal description?



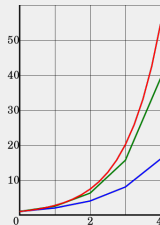
CONCRETE PICTURES OF WHAT WE WILL DO

What does a numerical solution look like?

t_0	t_1	t_2	t_3	\dots
x_0	x_1	x_2	x_3	\dots



(A) Slope field



(B) Solutions of $x' = x$, $x(0) = x_0$.
Euler (blue, bottom), Midpoint (green, middle), True (red, top)

- A numerical solution is a list of point values.
- (A) Each curve is a solution to IVP with a different initial value.
- (B) For each IVP, you have different numerical solutions depending on the method used.

Numerical solution of ODE

Taylor-series method

TAYLOR-SERIES METHOD

Setting/Notation

- Final time: T
- Uniform time steps: $h = (T - t_0)/N$ (N is #time steps),
 $t_n = t_0 + nh$ ($n = 0, 1, \dots, N$)
- x_n : numerical solution at t_n . We hope/expect $x_n \approx x(t_n)$.

How to approximate the next step computed? \rightarrow Taylor series

To compute $x(t + h)$, take a few terms from

$$x(t + h) = x(t) + hx'(t) + \frac{h^2}{2!}x''(t) + \frac{h^3}{3!}x'''(t) + \frac{h^4}{4!}x^{(4)}(t) + \dots$$

Example: 4th order Taylor method

$$\begin{cases} x'(t) = f(t, x) = \cos t - \sin x + t^2 \\ x(-1) = 3 \end{cases}$$

Numerical example desired.

- Problem of interest

$$\begin{cases} \dot{x} = f(t, x) \\ x(t_0) = x_0 \end{cases}$$

- Note carefully
 $x_n \neq x(t_n)$ in general.
- Taylor-series method is hard to summarize as a neat formula.

ERROR OF TAYLOR-SERIES METHOD

For example, if the method include up to 3rd order term, the error is of 4th order.

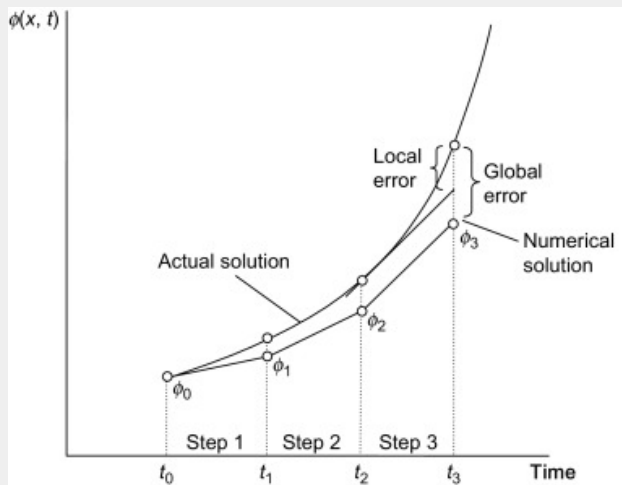
$$\underbrace{x(t+h)}_{\text{target}} - \underbrace{x(t) + hx'(t) + \frac{h^2}{2!}x''(t) + \frac{h^3}{3!}x'''(t) + \frac{h^4}{4!}x^{(4)}(t)}_{\text{approximation}} = \frac{h^5}{5!}x^{(5)}(\xi)$$

SOME STANDARD ONE-STEP METHOD OF NON-TAYLOR TYPE

- **Explicit Euler method:** (take first two terms from Taylor series.) $x_{n+1} = x_n + hf(t_n, x_n)$
 - **Implicit Euler:** $x_{n+1} = x_n + hf(t_{n+1}, x_{n+1})$
 - **Midpoint rule:** $x_{n+1} = x_n + hf\left(t_n + \frac{h}{2}, \frac{1}{2}(x_n + x_{n+1})\right)$
 - **Trapezoidal rule:** $x_{n+1} = x_n + \frac{h}{2}(f(t_n, x_n) + f(t_{n+1}, x_{n+1}))$
- **Question:** Guess the order of accuracy.
 - Explicit Euler method is actually a Taylor-series method.
 - Input of midpoint rule is the center of rectangle.
 - Trapezoidal rule is actually related to trapezoidal (quadrature) rule.
 - **Subjective question:** If you have an IVP, how would you choose a method? What would you consider?

ERRORS IN A NUMERICAL SOLUTION TO AN IVP

1. **Local truncation error (LTE)** : errors caused by including only finite number of calculations out of an exact procedure assuming the current data is exact.
 2. **Local roundoff error**: errors caused by limited precision of computers.
 3. **Global truncation error**: accumulation of all LTE. Usually, global error is of one lower order than that of LTE since errors accumulate.
 4. **Global roundoff error**: accumulated roundoff errors.
 5. **Total error**: sum of the global truncation errors and global roundoff errors.
- 'global error' usually means global truncation error. But people normally say the full name for 'local truncation error.'
 - Truncation errors are inherent in the method chosen, and quite independent of the roundoff errors.
 - Roundoff errors depend on the computer environment.



PROS AND CONS OF TAYLOR-SERIES METHOD

Pros

- Conceptually easy.
- High order methods are obtained easily (just add more terms).
- Inspires other methods.

Cons

- Require a high regularity on the slope function.
- Preliminary analytic work must be done. (During this stage, human-made error can be a disaster.)

Numerical solution of ODE

Runge-Kutta method

RUNGE-KUTTA METHOD

Motivation: In Taylor method, we need to find derivatives prior to coding. Can we reduce the human involvement?

Example: Derive a second order RK method (Board work).
Temporary notation (omitted evaluation) $x = x(t)$ and $f = f(t, x)$
(similarly for f_t, f_x, \dots)

1. Advance one step using Taylor's method.

$$x(t+h) = x(t) + hx'(t) + \frac{h^2}{2!}x''(t) + \frac{h^3}{3!}x'''(t) + \frac{h^4}{4!}x^{(4)}(t) + \dots$$

2. Replace derivatives of x with those (partial derivatives) of f .
For this, assume $x(t)$ solves the ODE $x'(t) = f(t, x(t))$.
3. Replace partials of f with only evaluations of f using Taylor series of $f(t+h, x+hf)$ in two variables.
4. Organize it.

- This leads to **Heun's method**.

$$\begin{aligned} x(t+h) \\ &= x(t) + \frac{1}{2}(F_1 + F_2), \end{aligned}$$

where

$$\begin{cases} F_1 = hf(t, x) \\ F_2 = hf(t+h, x+F_1). \end{cases}$$

RUNGE-KUTTA METHOD

Heun's method is not the only such methods. Every time we choose appropriate numbers for α, β, w_1, w_2 below, we have a method of order 2 (i.e., order 3 for one step):

$$\begin{aligned}x(t+h) &= x + w_1 hf + w_2 hf(t + \alpha h, x + \beta hf) + \mathcal{O}(h^3) \\&= x + w_1 hf + w_2 h[f + \alpha hf_t + \beta hff_x] + \mathcal{O}(h^3)\end{aligned}$$

Recall Taylor expansion of x requires

$$x(t+h) = x + \frac{1}{2}hf + \frac{1}{2}h[f + hf_t + hff_x] + \mathcal{O}(h^3).$$

We have a method of order 2 if

$$w_1 + w_2 = 1, \quad w_2\alpha = \frac{1}{2}, \quad w_2\beta = \frac{1}{2}.$$

$w_1 = 0, w_2 = 1, \alpha = \beta = \frac{1}{2}$ yield **modified Euler** method.

The previous observation motivates Butcher's tableau for RK method. A RK method can be encapsulated by

$$\begin{array}{c|cccc}
 c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\
 c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
 \hline
 & b_1 & b_2 & \cdots & b_s
 \end{array} = \begin{array}{c|c}
 \vec{c} & A \\
 \hline
 & \vec{b}^T
 \end{array}$$

Previous examples read:

$$\begin{array}{c|cc}
 0 & & \\
 1 & 1 & \\
 \hline
 & 1/2 & 1/2
 \end{array}$$

Heun's method

$$\begin{array}{c|cc}
 0 & & \\
 1/2 & 1/2 & \\
 \hline
 & 0 & 1
 \end{array}$$

modified Euler

- $\vec{b} \leftrightarrow$ weights of mid-stage slopes for the final advance (w 's)
- $\vec{c} \leftrightarrow$ time subgrid for stages (α)
- $A \leftrightarrow$ inner weights (β) for x as an input for mid-stage slopes.
- To yield a meaningful method, \vec{b}, \vec{c}, A must satisfy some requirements.
- We don't pursue detailed investigations on RK methods.

Runge-Kutta method decides the next step based on weighted average of the slopes at different locations in (t, x) -plain.

An important example: *The RK4*

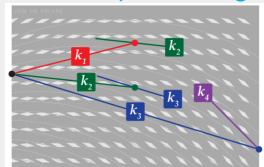
0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	0	$\frac{1}{2}$		
1	0	0	1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

or

$$\begin{cases} F_1 = hf(t, x) \\ F_2 = hf\left(t + \frac{1}{2}h, x + \frac{1}{2}F_1\right) \\ F_3 = hf\left(t + \frac{1}{2}h, x + \frac{1}{2}F_2\right) \\ F_4 = hf(t + h, x + F_3) \end{cases}$$

$$x(t + h) = x(t) + \frac{1}{6} (F_1 + 2F_2 + 2F_3 + F_4)$$

- Runge-Kutta methods from a slope field angle



- Subjective question:**
How would you summarize Runge-Kutta method in an intuitive language?