Math 104A - Intro to Numerical Analysis

Numerical Solution of ODE

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Intro

Problem of interest

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

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

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

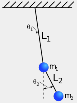
$$\vec{x}(t) = \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} \text{ and } f(t, x, y, z) = \begin{bmatrix} \sigma(y - x) \\ x(\rho - z) - y \\ xy - \beta z \end{bmatrix}$$

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

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

- $\dot{(\ )}$ denotes time derivative $\frac{\mathrm{d}}{\mathrm{dt}}(\ )$.
- $\vec{f}$ 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

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

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

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 $t\in[a,b]$,

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

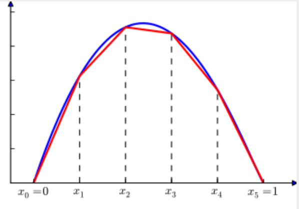
the (IVP) *has a unique solution on $[a,b]$.*

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

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

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

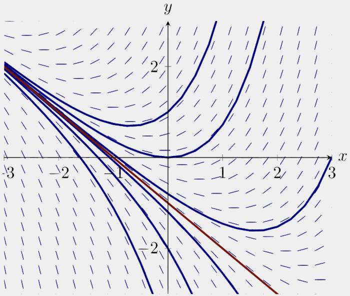
- To make the statement true, we end up needing to classify functions finer and finer.
- **Subjective question**: Lipschitz functions are very important class. Would you come up with a more intuitive, informal description?



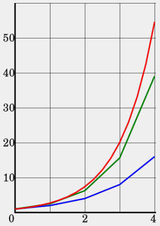
Concrete pictures of what we will do

What does a numerical solution look like?

t_0	t_1	t_2	t_3	$\cdots$
x_0	x_1	x_2	x_3	$\cdots$



(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), $t_n = t_0 + nh$ ($n = 0, 1, \cdots, N$)
- x_n: numerical solution at t_n. We hope/expect $x_n \approx x(t_n)$.

How to approximate the next step computed? → Taylor series
To compute $x(t+h)$, take a few terms from

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

Example: 4th order Taylor method

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

- 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

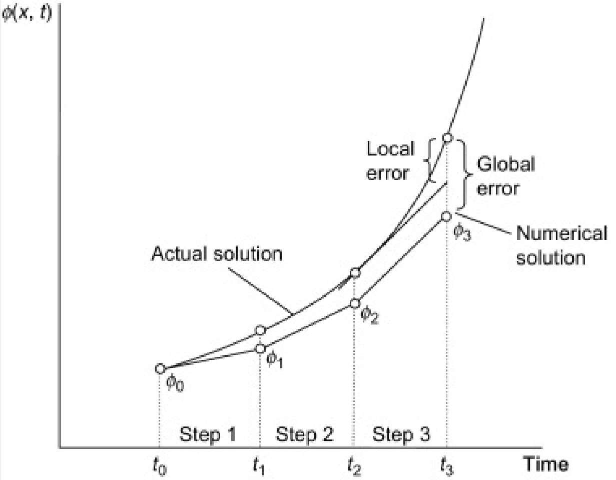
- **Explicit Euler method**: (take first two terms from Taylor series.) $x_{n+1} = x_n + hf(t_n, x_n)$
- **Implicit Euler**: $x_{n+1} = x_n + hf(t_{n+1}, x_{n+1})$
- **Midpoint rule**: $x_{n+1} = x_n + hf\left(t_n + \frac{h}{2}, \frac{1}{2}(x_n + x_{n+1})\right)$
- **Trapezoidal rule**: $x_{n+1} = x_n + \frac{h}{2}\left(f(t_n, x_n) + f(t_{n+1}, x_{n+1})\right)$

- **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 from a single step advance that is 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.


$\phi(x, t)$
Local error
Global error
Numerical solution
Actual solution
ϕ_0
ϕ_1
ϕ_2
ϕ_3
Step 1
Step 2
Step 3
t_0
t_1
t_2
t_3
Time

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

Before we begin

- Putting off ComHW2 to Thu (Dec 1) and moving Fri OH 4:10-5:10PM to Wed 12:00-1:00PM.
- Join ESCI!! You can also leave comments on iclicker.
- Some answers to "How would you choose a method for IVPs?" (11AM)
    - Based on initial conditions and how accurate I must be. But if I can get it done easily I'm using explicit euler if else I'll se trapezoida
    - Depending on the context and the goal of accuracy and computation power needed.
    - I would use the explicit euler method to solve. it is the quickest/simplest one to solve as it requires the least amount of computation.
    - If I have an IVP, I would see the function form and decide the solving method. To see if it is separable or replaceable?
    - how difficult xn+1 is to calculate in terms of f like if it is easy or hard to find the root for the implicit versions
    - it would depend on how annoying f is. the bigger it is the harder to solve for xn+1
    - It depends on what what nodes are provided to you.

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 $f_t, f_x, \cdots$)

1. Advance one step using Taylor's method.
$$x(t+h) = x(t) + hx'(t) + \frac{h^2}{2!}x''(t) + \frac{h^3}{3!}x'''(t) + \frac{h^4}{4!}x^{(4)}(t) + \cdots$$
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):

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

Recall Taylor expansion of x requires

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

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.

Butcher's tableau for Runge-Kutta method

The previous observation motivates Butcher's tableau for RK method. An 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:

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

Heun's method   modified Euler

Activity: Recover modified Euler from the tableau.

- $\vec{b} \leftrightarrow$ 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.

“best” Runge-Kutta method

Irregular accuracy of RK

# function eval.	1	2	3	4	5	6	7	8
Max order of accuracy	1	2	3	4	4	5	6	6

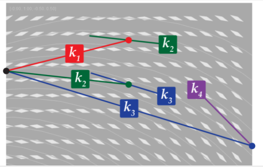
An important example: *The (classical)* RK4

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

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

Activity: Construct Butcher's tableau for the RK4.

- Runge-Kutta methods from a slope field angle



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

Optional computational project

Simulate the Lorenz system with several method and compare the trajectories. (explicit Euler, implicit Euler, RK4)

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

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

- Consider changing the initial condition. I have chosen it randomly.

Numerical solution of ODE

Multistep Methods

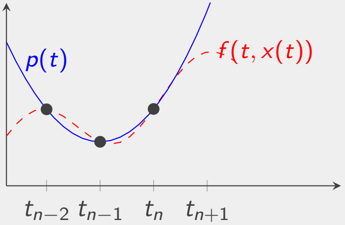
Multistep methods

Single-step methods: Taylor and RK methods use only the data at the most recent time grid: find x_{n+1} given x_n at t_n.

Multistep methods: The methods use more history: find x_{n+1} given $x_n, x_{n-1}, \cdots, x_{n-k+1}$ at $t_n, t_{n-1}, \cdots, t_{n-k+1}$.

- Don't get confused with 'stages.' RK4, for example, uses four different mid-stage slopes which the method *computes* but not *given*.

Multistep methods - Adam-Bashforth



Idea: use interpolation and quadrature ($k=3$, uniform grid)

1. Suppose x solves the ODE, $x' = f(t,x)$, and integrate

$$x\left(t_{n+1}\right) = x\left(t_n\right) + \int_{t_n}^{t_{n+1}} x'(t)dt = x\left(t_n\right) + \int_{t_n}^{t_{n+1}} f(t,x(t))dt$$

2. Replace $f(t,x(t))$ with its polynomial interpolation $p(t)$ at $(t_{n-2}, f_{n-2}), (t_{n-1}, f_{n-1}), (t_n, f_n)$, where $f_j := f(t_j, x(t_j))$.
3. Obtain a method by labeling $x_j \approx x(t_j)$. It should be clear that

$$x_{n+1} = x_n + Af_n + Bf_{n-1} + Cf_{n-2}$$

- Question: What is the degree of $p(t)$?
- Question: Write out $p(t)$.

Example: Derive 3 step Adam-Bashforth method (AB3)

$$x_{n+1} = x_n + h\left(\frac{23}{12}f_n - \frac{16}{12}f_{n-1} + \frac{5}{12}f_{n-2}\right)$$

- **Subjective question**: What can be a quick sanity check?

Order of Adam-Bashforth methods

Theorem

LTE of k–step AB method is of order $k+1$, that is, $|x_{n+1} - x(t_{n+1})| = \mathcal{O}\left(h^{k+1}\right)$ *as* $h \to 0$.

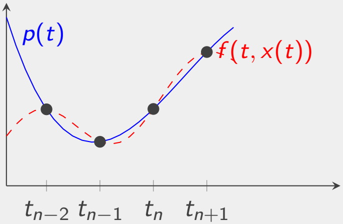
Proof.

Board Work. □

- Recall: Let $x_0, x_1, \cdots, x_n \in [a,b]$ be distinct nodes, $f \in C^{n+1}[a,b]$, and $p \in \Pi_n$ interpolating f at the nodes. For each $x \in [a,b]$, there is $\xi_x \in (a,b)$ such that

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)$$

Multistep methods - Adam-Moulton



Same Idea: use interpolation and quadrature ($k = 3$, uniform grid)

1. Suppose x solves the ODE, $x' = f(t, x)$, and integrate

$$x(t_{n+1}) = x(t_n) + \int_{t_n}^{t_{n+1}} x'(t)dt = x(t_n) + \int_{t_n}^{t_{n+1}} f(t, x(t))dt$$

2. Replace $f(t, x(t))$ with its polynomial interpolation $p(t)$ at $(t_{n-2}, f_{n-2}), (t_{n-1}, f_{n-1}), (t_n, f_n), (t_{n+1}, f_{n+1})$. ($f_j := f(t_j, x(t_j))$)
3. Obtain a method by labeling $x_j \approx x(t_j)$:

$$x_{n+1} = x_n + Af_{n+1} + Bf_n + Cf_{n-1} + Df_{n-2}$$

- Question: What is the degree of $p(t)$?

Multistep methods - Adam-Moulton

Example: 3 step Adam-Moulton method (AM3)

$$x_{n+1} = x_n + h\left(\frac{9}{24} f\left(t_{n+1}, x_{n+1}\right) + \frac{19}{24} f\left(t_n, x_n\right) - \frac{5}{24} f\left(t_{n-1}, x_{n-1}\right) + \frac{1}{24} f\left(t_{n-2}, x_{n-2}\right)\right)$$

- Question: Is this possible?
- Question: Guess the order of accuracy.

Adam-Moulton method equipped with an iterative method

Issue: We need to know x_{n+1} to compute x_{n+1}! (Implicit)

$$x_{n+1} = x_n + h\left(\frac{9}{24}f\left(t_{n+1}, x_{n+1}\right)\right.$$
$$\left. + \frac{19}{24}f\left(t_n, x_n\right) - \frac{5}{24}f\left(t_{n-1}, x_{n-1}\right) + \frac{1}{24}f\left(t_{n-2}, x_{n-2}\right)\right)$$

Idea: Recast the method as a fixed point problem.

1. Relabel what we are after, x_{n+1}, say, z to emphasize that it is the real unknown.

2. Treat everything else, which is already known, as data and lump it into a single function, say, ϕ.

3. Find the solution, z such that

$$z = \phi(z) := C_1 hf(t_{n+1}, z) + C2.$$

That is, $z_{m+1} = \phi(z_m)$ for $m = 0, 1, 2, \cdots$.

Accuracy of Adam-Moulton method

Theorem

LTE of k–step AM method is of order $k+2$, that is,
$|x_{n+1} - x(t_{n+1})| = \mathcal{O}\big(h^{k+2}\big)$ *as* $h \to 0$.

Proof.

Board Work. □

Predictor-Corrector method

Issue: We need to know x_{n+1} to compute x_{n+1}! (Implicit)
Idea: Make an explicit variant of Adam-Moulton method.

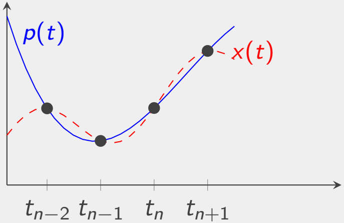
1. Choose one Adam-Bashforth method of one more step. (e.g, choose AB4 if AM3 is the main method).
2. Run the AB method (explicit) to *predict* the next x value, call it x^*_{n+1}.
3. Run the AM method using the predicted value on RHS in $f(t_{n+1}, x^*_{n+1})$ instead of $f(t_{n+1}, x_{n+1})$ to *correct* the prediction.

That is, if AM3 is the main method,

$$x_{n+1} = x_n + h\left(\frac{9}{24} f\left(t_{n+1}, x^*_{n+1}\right) + \frac{19}{24} f\left(t_n, x_n\right) - \frac{5}{24} f\left(t_{n-1}, x_{n-1}\right) + \frac{1}{24} f\left(t_{n-2}, x_{n-2}\right)\right).$$

- The rationale behind this is to keep the same order of accuracy. Since AB4 involves four coefficients for $f_n, f_{n-1}, f_{n-2}, f_{n-3}$, our intuition says it is of order 4. On the other hand, AM3 involves four coefficients for $, f_{n+1}, f_n, f_{n-1}, f_{n-2}$. Otherwise, you loose accuracy for no reason.

Backward differentiation formula (BDF)



Motivation: The methods of Adam's family are based on interpolating the slope functions. Can we obtain interpolating positions, x's?

1. Given x_{n-2}, x_{n-1}, x_n at t_{n-2}, t_{n-1}, t_n resp., pretend to know x_{n+1} at t_{n+1} and find a polynomial $p(t)$ interpolating the four points.
2. Assume $x'(t) \approx p'(t)$, and argue $p'(t_{n+1}) \approx x'(t_{n+1}) = f_{n+1}$.

- Recall, from numerical differentiation, this approximation is really true if the solution is smooth enough.
- It literally looks backwards come up with a formula for the numerical differentiation.

Backward differentiation formula (BDF)

Examples:

$$\begin{aligned}
&\text{BDF1} & x_{n+1} - x_n &= hf_{n+1} \\
&\text{BDF2} & x_{n+1} - \tfrac{4}{3}x_n + \tfrac{1}{3}x_{n-1} &= \tfrac{2}{3}hf_{n+1} \\
&\text{BDF3} & x_{n+1} - \tfrac{18}{11}x_n + \tfrac{9}{11}x_{n-1} - \tfrac{2}{11}x_{n-2} &= \tfrac{6}{11}hf_{n+1}
\end{aligned}$$

- BDF methods are all implicit. Recall $f_{n+1} := f(t_{n+1}, x_{n+1})$.
- In some sense, BDF methods are “dual” to Adam’s family: BDF minimizes #slope evaluations while Adam’s #history of x’s
- BDFs are considered good option for ‘stiff’ problem. (This notion makes sense only in high dimensions.)

Linear multistep method

$$\sum_{i=1}^{k+1} a_i x_i = h \sum_{i=1}^{k+1} b_i f_i$$

- Adam-Bashforth: $a_{k+1} = 1, a_k = -1$; all other a's are zero; $b_{k+1} = 0$; other b's are appropriately chosen
- Adam-Moulton: $a_{k+1} = 1, a_k = -1$; all other a's are zero; $b_{k+1} \neq 0$; other b's are appropriately chosen
- BDF: $b_{k+1} \neq 0$; other b's are zero; all a's are chosen appropriately
- In theory, we can make the most out of the degrees of freedom by tuning a's and b's to obtain as accurate method as possible. But we will see the method of the highest possible order is not a good option.

- There are many other linear multistep methods.
- **Question**: Guess how high the order of the method can be.

Topics with Incomplete treatment

Important facts but that are tricky to discuss.

- **Dahlquist Equivalence theorem**: convergence = stability + consistency
- **Dahlquist first barrier**: the order of a stable and linear k-step method cannot be $> k+1$ if k is odd and $> k+2$ if k is even. If the method is explicit, then it cannot be $> k$.
- **Dahlquist second barrier** (not covered; relevant in multi-dimensions): no explicit linear multistep methods are A-stable. Further, the maximal order of an (implicit) A-stable linear multistep method is 2.
- **Order of global truncation error**: LTE $= \mathcal{O}\big(h^{m+1}\big) \implies$ GTE $= \mathcal{O}\big(h^m\big)$.

What we will focus on

- Dahlquist Equivalence theorem: (a) Motivation for stability and the definition of convergence (consistency is very natural). (b) We don't prove this.
- Dahlquist first barrier: Just accept this. Its proof is esoteric.
- Dahlquist second barrier: Just mention this. We didn't cover high dimensional setting. Even if we did, its proof is esoteric.
- Order of global truncation error: I mentioned a "wrong" proof. A rigorous treatment requires quite a bit of preparations.

Order of Linear Multistep method

Definition

Given a linear multistep method $\sum_{i=0}^{k} a_i x_i = h \sum_{i=0}^{k} b_i f_i$, define the linear operator $L : C^1 \to \mathbb{R}$ associated to the method

$$L[y] = \sum_{i=0}^{k} a_i y(ih) - h \sum_{i=0}^{k} b_i y'(ih).$$

- $h > 0$ is a fixed time step size.
- **Notation**: From now on, we change the index convention so that $i = 0, 1, 2, \cdots, k$ for convenience.
- I am going to call L *error* or *residual* operator (or functional). This is not a standard name.

Order of Linear Multistep method

Define

$$d_0 = \sum_{i=0}^{k} a_i$$

$$d_1 = \sum_{i=0}^{k} (ia_i - b_i)$$

$$d_2 = \sum_{i=0}^{k} \left(\frac{1}{2} i^2 a_i - ib_i \right)$$

$$\vdots$$

$$d_j = \sum_{i=0}^{k} \left(\frac{i^j}{j!} a_i - \frac{i^{j-1}}{(j-1)!} b_i \right) \quad (j \geq 1)$$

Order of Linear Multistep method

Theorem (Order condition)

The following are equivalent:

1. *The LTE of linear multistep method* $\sum_{i=0}^{k} a_i x_i = h \sum_{i=0}^{k} b_i f_i$ *is of order* $m+1$*.*
2. $d_0 = d_1 = \cdots = d_m = 0$
3. $L[y] = \mathcal{O}\left(h^{m+1}\right)$ *for all* $y \in C^{m+1}$*, where* L *is the linear operator associated with the method:* $L[y] = \sum_{i=0}^{k} a_i y(ih) - h \sum_{i=0}^{k} b_i y'(ih)$*.*

- LTE in words: *how much the true solution fail to satisfy the method.*
- If $L[y] = \mathcal{O}\left(h^{m+1}\right)$ with $m \geq 1$, we say it is **consistent** (to order m). That is, it discretizes the ODE $x' = f(t, x)$ in a consistent manner: the formula approaches the ODE as $h \to 0$.
- For this reason, order of LTE is also called **consistency order**.

Convergence theory for linear multistep methods

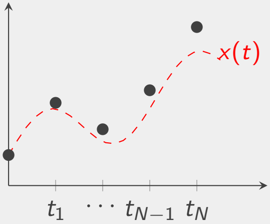
A complete treatment of consistency, stability and convergence requires quite a bit of preparations. So, we only glimpse at the big picture and learn important results.

Definition

A k–step method is said to be convergent if

$$\max_{0\leq i\leq N} \{|x_i - x(t_i)|\} \to 0 \text{ as } h \to 0$$

whenever the initial values satisfy $\max_{0\leq i\leq k-1}\{|x_i - x(t_i)|\} \to 0$ as $h \to 0$.



- Recall: $h = T/N$ (time step size), $t_i = hi$ (i-th time grid), $x(t_i)$ is the true solution evaluated at t_i, x_i is an approximation of $x(t_i)$ using the method chosen.

Convergence theory for linear multistep methods

Motivating example: Some 3-step method, denoted by S for 'scheme,' is used to solve an IVP and see what happens to the first approximation.

$$x_3 = S(x_0, x_1, x_2, h)$$
$$x(t_3) = S(x(t_0), x(t_1), x(t_2), h) + \tau_3[x].$$

Subtracting and labeling errors $e_i = x_i - x(t_i)$,

$$e_3 = z_3 + \tau_3[x],$$

where z_3 represent the error propagated by feeding wrong initial values (recall that only $x_0 = x(0)$ is guaranteed). Let's advance one more step for intuition.

$$x_4 = S(x_1, x_2, x_3, h)$$
$$x(t_4) = S(x(t_1), x(t_2), x(t_3), h) + \tau_4[x]$$

Thus,

$$e_4 = z_4 + \tau_4[x]$$

- **Advice**: When notation is heavy, it is often helpful to call them assigning meanings. E.g., $\tau_3[x]$ represents (t)runcation error at step (3) for the true solution x.
- In z_3, 'z' for error related to zero-stability

Convergence theory for linear multistep methods

Emphasizing dependence of this error,

$$e_4 = z_4(e_1, e_2, e_3) + \tau_4[x] = z_4(e_1, e_2, z_3(e_1, e_2), \tau_3[x]) + \tau_4[x]$$

Lesson: The global error is not merely a sum of truncation errors, but it is a result of interactions of the local truncation errors and error propagation due to inexact initial data fed each step of the method.

$$\begin{aligned} e_5 &= z_5(e_2, e_3, e_4) + \tau_5[x] \\ e_4 &= z_4(e_1, e_2, e_3) + \tau_4[x] \\ e_3 &= z_3(e_0, e_1, e_2) + \tau_3[x] \end{aligned}$$

Strategy: Establish (a) z_n is small if e_{n-2}, e_{n-1}, e_n are small, and (b) $\tau_n[x]$ is small if h is small. These two combine to give us e_n is small for all $n = 1, 2, \cdots, N$, at least morally.

- To ensure convergence, we need to have both conditions.
- (a) is related to (zero-)**stability**, and (b) to **consistency**.
- If you use a method of order ≥ 1, then the consistency is fulfilled ✓(b). But there is simpler way to check this.

Zero-stability

Definition (Zero-stability)

A linear k–step method is **zero-stable** if there is a constant C such that, for any $\{x_i\}$ and $\{y_i\}$ that have been generated by the same method but with different initial values $x_0, x_1, \cdots, x_{k-1}$ and $y_0, y_1, \cdots, y_{k-1}$ respectively, we have

$$|x_n - y_n| \leq C \max\{|x_0 - y_0|, \cdots, |x_{k-1} - y_{k-1}|\}$$

for all $n \leq N$, where N is the last time index for the final time of an IVP: $T = hN$.

There is a much simpler way to check whether a method has this property. We need several tools for that.

- In words, a (zero-) stable method does not amplify the error (in the initial conditions).

Zero-stability

Definition (Characteristic polynomials)

The first and second characteristic polynomials associated with a k–step method $\sum_{i=0}^{k} a_i x_i = h \sum_{i=0}^{k} b_i f_i$ is given by

$$p(z) = \sum_{i=0}^{k} a_i z^i \quad \text{and} \quad q(z) = \sum_{i=0}^{k} b_i z^i$$

Example: find characteristic polynomials of BDF2

Definition (Root condition)

A polynomial $p(z)$ of degree k is said to satisfy the **root condition** if its roots are in the closed unit circle $\{z \in \mathbb{C} \ : \ |z| \leq 1\}$ and any roots of modulus 1 is simple.

Zero-stability

Theorem

A linear k-step method is zero-stable if and only if its first characteristic polynomial satisfies the root condition.

Proof.

See Endre Süli and David F. Mayers. *An introduction to numerical analysis*. Cambridge University Press, Cambridge, 2003, pp. x+433. ISBN: 0-521-81026-4; 0-521-00794-1, Theorem 12.4. □

Strategy: Establish ✓(a) z_n is small if e_{n-2}, e_{n-1}, e_n are small, and (b) $\tau_n[x]$ is small if h is small. These two combine to give us e_n is small for all $n = 1, 2, \cdots, N$, at least morally.

- Many textbooks, including our own, define the zero-stability of a linear multistep method through the root condition.
- Checking the root condition completes a half of our strategy.

Consistency

Theorem

Let $p(z)$ and $q(z)$ are the first and second characteristic polynomials of a multistep method. If

$$p(1) = 0 \text{ and } p'(1) = q(1),$$

then the LTE of the method is of order m with $m \geq 1$.

Strategy: Establish (a) z_n is small if e_{n-2}, e_{n-1}, e_n are small, and ✓(b) $\tau_n[x]$ is small if h is small. These two combine to give us e_n is small for all $n = 1, 2, \cdots, N$, at least morally.

Convergence of linear multistep method

Theorem (Dahlquist equivalence theorem)

A multistep method is convergent iff it is stable and consistent.

Theorem (Global order of convergence)

If the LTE of a convergent multistep method is $\mathcal{O}\left(h^{m+1}\right)$ as $h \to 0$, then the global truncation error of the method is $\mathcal{O}\left(h^{m}\right)$ as $h \to 0$.

Theorem (Dahlquist first barrier)

The order of a stable and linear k-step method cannot be higher than $k+1$ if k is odd or than $k+2$ if k is even. If the method is explicit, then it cannot be greater than k.

- Therefore, to show convergence, one needs to check (a) root condition and (b) consistency condition $p(1) = 0$ and $p'(1) = q(1)$.

Convergence of linear multistep method

Example

Show the explicit Euler is convergent.

Example

Show the AB3 is convergent.

- **Question**: What does this mean? (Explicit Euler is convergent.)