ESS101- Modeling and Simulation
Lecture 18-19

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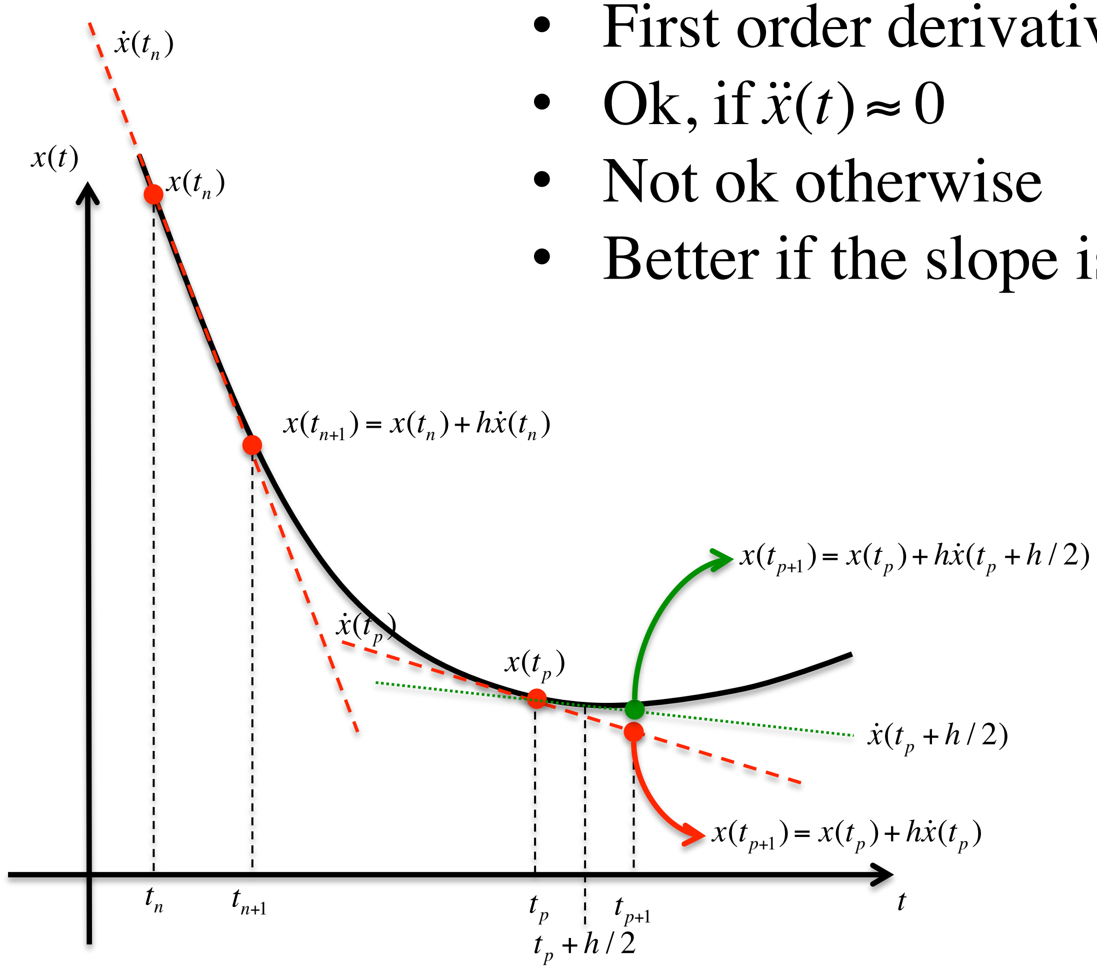
Today (Chapters 9, 10)

- ☞ Motivating example
- ☞ General RK methods
- ☞ Four multi-stage RK methods
- ☞ Absolute stability of RK methods

Motivating example



Remarks

- First order derivative used
- Ok, if $\ddot{x}(t) \approx 0$
- Not ok otherwise
- Better if the slope is “sampled” finer

Numerical Example

Simulate the system

$$\dot{x}(t) = (1-2t)x(t), \quad x(0) = 1$$

$$0 \le t \le 1.2$$

Recall the ***exact solution*** $x(t) = e^{\frac{1}{4}-\left(\frac{1}{2}-t\right)^2}$

Calculate the approximate solution as

$$x_{n+1} = x_n + h\dot{x}_n \quad \text{(FE)}, \rightarrow x_{n+1} = x_n + hk_2,$$

$$k_2 = \dot{x}\left(t_n + \frac{1}{2}h\right) = \left(1-2t_n - h\right)x\left(t_n + \frac{1}{2}h\right)$$

$$x\left(t_n + \frac{1}{2}h\right) \approx x_n + \frac{h}{2}\dot{x}_n$$

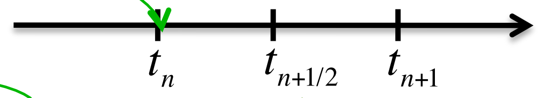
Numerical Example

The n-th iteration is

$$k_1 = f\left(t_n, x_n\right) \quad \text{(slope)}$$

$$k_2 = f\left(t_n + \frac{1}{2}h, x_n + \frac{1}{2}hk_1\right) \quad \text{(slope)}$$

$$x_{n+1} = x_n + hk_2, \quad \text{(solution)}$$



GE*10^3@t=1.2

h	TS(2)	Trap.	ABE	ABT	RK(2)
0.2	5.4	−2.8	−3.6	17.6	3.5
0.1	1.4	−0.71	−0.66	4.0	0.67
Ratio	3.90	4.00	5.49	4.40	5.24

2nd order methods

General RK methods

The n-th iteration of a ***s-stage*** method is

$$x_{n+1} = x_n + h\sum_{i=1}^{s} \underbrace{b_i}_{\text{weights}} k_i,$$

Weighted linear combination of slopes in $[t_n, t_{n+1}]$

$$k_i = f\left(t_n + c_i h,\; x_n + h\sum_{j=1}^{s} a_{i,j} k_j\right), \quad i = 1,\ldots,s$$

solution at $t_n + c_i h$

Pick points in $[t_n, t_{n+1}]$ where slopes are calculated

slopes at $t_n + a_{i,j} h$

t_n $\quad t_n + a_{i,1}h \quad \cdots \quad t_n + a_{i,i-1}h \quad t_n + c_i h \quad t_{n+1}$

slope calculated here

Hence, natural choices for c_i and $a_{i,j}$ are

$$c_i = \sum_{j=1}^{s} a_{i,j}, \quad i = 1,\ldots,s \qquad\qquad a_{i,j} = 0, \quad j \ge i$$

General RK methods

$$
\begin{array}{c|cccc}
c_1 & a_{1,1} & a_{1,2} & \cdots & a_{1,s} \\
c_2 & a_{2,1} & a_{2,2} & \cdots & a_{2,s} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
$$

Butcher array for a full RK method (implicit)

$$
\begin{array}{c|cccc}
0 & 0 & 0 & \cdots & 0 \\
a_{2,1} + a_{2,2} & a_{2,1} & a_{2,2} & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\sum_{j=1}^{s} a_{s,j} & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
$$

Butcher array for an explicit RK method

For a s-*stage* method s^2+s parameters $(a_{i,j}, b_i)$ must be determined. How?

With fixed s, maximize the method order

One-stage methods

A s-stage method is of order p if

$$e_{n+1} = x(t_{n+1}) - x_{n+1} = O(h^{p+1})$$

Recall the e_{n+1} is the local error. That is, calculated by assuming $x(t_n)=x_n$

For $s=1$ $\quad x_{n+1} = x_n + hb_1k_1 \qquad k_1 = f\left(t_n + c_1h, x_n + a_{1,1}k_1\right)$

$$= \Big|_{\substack{c_1=0 \\ a_{1,1}=0}} f\left(t_n, x_n\right)$$

To form the local error let's expand $x(t_{n+1})$ is Taylor series

$$x\left(t_{n+1}\right) = x\left(t_n\right) + h\dot{x}\left(t_n\right) + \frac{1}{2!}h^2\ddot{x}\left(t_n\right) + O(h^3)$$

where $\ddot{x}\left(t_n\right)$ is calculated as $\ddot{x}\left(t_n\right) = \frac{\partial}{\partial t} f(t_n, x_n) + \dot{x}\left(t_n\right)\frac{\partial}{\partial x} f(t_n, x_n)$

One-stage methods

Hence $x(t_{n+1}) = x(t_n) + h\dot{x}(t_n) + \frac{1}{2!}h^2\left[f_t + \dot{x}(t_n)f_x\right] + O(h^3)$

The expression of the local error is

$$e_{n+1} = x(t_{n+1}) - x_{n+1}$$

$$= x(t_n) + h\dot{x}(t_n) + \frac{1}{2!}h^2\left[f_t + \dot{x}(t_n)f_x\right] - x(t_n) - hb_1 \underbrace{\overbrace{f\left(t_n, x(t_n)\right)}^{k_1}}_{\dot{x}(t_n)} + O(h^3)$$

$$= h(1-b_1)\dot{x}(t_n) + \frac{1}{2!}h^2\left[f_t + \dot{x}(t_n)f_x\right] + O(h^3)$$

The maximum attainable order is $p=1$ with $b_1=1$

$x_{n+1} = x_n + hk_1 \qquad k_1 = f(t_n, x_n)$ ***FE Euler method***

Two-stage methods

For ***s=2*** the *n*-th iteration is

$$
\begin{aligned}
x_{n+1} &= x_n + h\left(b_1 k_1 + b_2 k_2\right),\\
k_1 &= f\left(t_n, x_n\right)\\
k_2 &= f\left(t_n + ah, x_n + ahk_1\right)
\end{aligned}
$$

Find a, b_1, b_2 to maximize the method order

To calculate the ***local error*** write the method with $x_n = x(t_n)$

$$
\begin{aligned}
x_{n+1} &= x\left(t_n\right) + h\left(b_1 f\left(t_n, x\left(t_n\right)\right) + b_2 f\left(t_n + ah, x\left(t_n\right) + ahf\left(t_n, x\left(t_n\right)\right)\right)\right)\\
&= x\left(t_n\right) + hb_1\dot{x}\left(t_n\right) + hb_2 f\left(t_n + ah, x\left(t_n\right) + ah\dot{x}\left(t_n\right)\right)\\
&= x\left(t_n\right) + hb_1\dot{x}\left(t_n\right) + hb_2\left(f\left(t_n, x\left(t_n\right)\right) + ah\frac{\partial}{\partial t} f\left(t_n, x\left(t_n\right)\right) + ah\dot{x}\left(t_n\right)\frac{\partial}{\partial x} f\left(t_n, x\left(t_n\right)\right) + O(h^2)\right)\\
&= x\left(t_n\right) + hb_1\dot{x}\left(t_n\right) + hb_2\left(\dot{x}\left(t_n\right) + ahf_t + ah\dot{x}\left(t_n\right) f_x + O(h^2)\right)
\end{aligned}
$$

Two-stage methods

To calculate the local error expand $x(t_{n+1})$ as

$$x(t_{n+1}) = x(t_n) + h\dot{x}(t_n) + \frac{1}{2!}h^2\left[f_t + \dot{x}(t_n)f_x\right] + \frac{1}{3!}h^3\dddot{x}(t_n) + O(h^4)$$

Calculate the local error e_{n+1} as

$$\begin{aligned}
e_{n+1} &= x(t_{n+1}) - x_{n+1} \\
&= x(t_n) + h\dot{x}(t_n) + \frac{1}{2!}h^2\left[f_t + \dot{x}(t_n)f_x\right] + \frac{1}{3!}h^3\dddot{x}(t_n) + O(h^4) \\
&\quad - x(t_n) - h(b_1 + b_2)\dot{x}(t_n) - hb_2\left(ahf_t + ah\dot{x}(t_n)f_x + O(h^2)\right) \\
&= h(1 - b_1 - b_2)\dot{x}(t_n) + h^2\left(\frac{1}{2} - ab_2\right)\left[f_t + \dot{x}(t_n)f_x\right] + \frac{1}{3!}h^3\dddot{x}(t_n) + O(h^4)
\end{aligned}$$

Two-stage methods

$$e_{n+1} = h\left(1 - b_1 - b_2\right)\dot{x}\left(t_n\right) + h^2\left(\frac{1}{2} - ab_2\right)\left[f_t + \dot{x}\left(t_n\right)f_x\right] + \frac{1}{3!}h^3\dddot{x}\left(t_n\right) + O(h^4)$$

By setting $b_1 + b_2 = 1$ the method has order ***p=1*** $\forall a$

By setting $b_1 + b_2 = 1$ and $ab_2 = \dfrac{1}{2}$ the method has order ***p=2***

Two conditions on *three parameters* for ***order two***

Q: Can one more condition be derived by expanding the method equations further to achieve order 3?

A: It can be shown (see p. 129) that there is not a combination of parameter enabling *p=3*

Three-stage methods

For ***s=3*** the *n*-th iteration is

$$x_{n+1} = x_n + h\left(b_1 k_1 + b_2 k_2 + b_3 k_3\right), \qquad k_2 = f\left(t_n + c_2 h, x_n + a_{2,1} h k_1\right)$$

$$k_1 = f\left(t_n, x_n\right) \qquad k_3 = f\left(t_n + c_3 h, x_n + a_{3,1} h k_1 + a_{3,2} h k_2\right)$$

Similarly to 2-stage methods, it can be shown that

$$b_1 + b_2 + b_3 = 1 \qquad \text{(order 1)}$$

$$b_2 c_2 + b_3 c_3 = \frac{1}{2} \qquad \text{(order 2)}$$

$$\left.\begin{aligned} b_2 c_2^2 + b_3 c_3^2 &= \frac{1}{3} \\ c_2 a_{3,2} b_3 &= \frac{1}{6} \end{aligned}\right\} \qquad \text{(order 3)}$$

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{3} & \frac{1}{3} & 0 & \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

Heun's 3rd order rule

$$\begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & \frac{1}{2} & 0 & \\ 1 & -1 & 2 & 0 \\ \hline & \frac{1}{6} & \frac{4}{3} & \frac{1}{6} \end{array}$$

RK's 3rd order rule

Four-stage methods

$$
\begin{array}{c|cccc}
0 & 0 & & & \\
\frac{1}{2} & \frac{1}{2} & 0 & & \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

Order s cannot be achieved for a s-step method with $s>4$

Higher step methods are impractical. Large number of equations to solve.

Absolute stability

Definition (Absolute stability). A RK method is ***absolutely stable*** if its solution x_n to the problem

$$\dot{x}(t) = \lambda x(t), \quad \mathrm{Re}(\lambda) < 0$$

converges to zero as $n \to \infty$

Example

Study the stability of a RK(2) with the following coefficients

$$x_{n+1} = x_n + h\left(b_1 k_1 + b_2 k_2\right),$$
$$k_1 = f\left(t_n, x_n\right)$$
$$k_2 = f\left(t_n + ah, x_n + ahk_1\right)$$

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2\theta} & \frac{1}{2\theta} & \\ \hline & 1-\theta & \theta \end{array}$$

(order 2 conditions)

Absolute stability

$$x_{n+1} = x_n + h\left(b_1 k_1 + b_2 k_2\right),$$
$$k_1 = f\left(t_n, x_n\right)$$
$$k_2 = f\left(t_n + ah, x_n + ahk_1\right)$$

$$\begin{array}{c|cc} 0 & 0 & \\ \frac{1}{2\theta} & \frac{1}{2\theta} & \\ \hline & 1-\theta & \theta \end{array}$$

The n-th iteration becomes

$$x_{n+1} = x_n + h\left(1-\theta\right)\lambda x_n + h\theta\left(\lambda x_n + \frac{\lambda^2 h}{2\theta} x_n\right)$$
$$= \left(1 + h\lambda + \frac{\lambda^2 h^2}{2}\right) x_n$$

The corresponding characteristic polynomial is

$$p(r) = r - \left(1 + h\lambda + \frac{\lambda^2 h^2}{2}\right) \qquad \Rightarrow \left|1 + h\lambda + \frac{\lambda^2 h^2}{2}\right| < 1$$ ***Stability condition***

Stability regions