Ordinary Differential Equations (I)

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Numerical Methods,
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Plan for today

- General problem of estimating the solution to an equation that involves some unknown function and its derivatives
    - What do we need to know to do this?
- Specific problems in which we know the initial condition for our function

Nomenclature and Preliminaries

We will discuss ordinary differential equations, or systems of linear ordinary differential equations:

differential equation
: Any equation of the form

$$F(x; y, y', y^{(2)}, \ldots, y^{(n)}) = 0$$

with $x \in \mathbb{R}$ and $y(x) : \mathbb{R} \mapsto \mathbb{R}^m$ is called a system of ordinary differential equations of order n.
If $m = 1$, it is only one ordinary diff. equation (ODE).

linear
: If we can write

$$F(x; y, \ldots, y^{(n)}) = A(x) \cdot \vec{y}(x) + r(x)$$

with $A(x) \in \mathbb{R}^{m \times (n+1)}$, $\vec{y}(x) = (y(x), \ldots y^{(n)}(x))^T$ and $r(x) \in \mathbb{R}^m$, then F describes a linear system of ODEs.

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ordinary The quality ordinary hinges on the fact that y only depends on $x \in \mathbb{R}$. As soon as $x \in \mathbb{R}^k$, and we need to consider partial derivatives of y, we have a partial differential equation.

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explicit If for an nth order ODE we can write

$$y^{(n)} = f(x; y, \ldots, y^{(n-1)})$$

then we call this an explicit ODE. Otherwise, the ODE is implicit.

Explicit linear ODEs of order $n = 1$/Initial value problem

Let's use a well-known linear ODE of 2nd order as an example:

$$y' = f(x; y) = -y(x)$$

Solving it, regardless of method, poses an initial value problem:

$$\frac{y(x)}{y(x_0)} = \exp(-(x - x_0)) \tag{1}$$

We need to know the initial value $y_0 \equiv y(x_0)$ to solve this problem. It must be provided externally.

Single Step Methods

We want to increment by one step, i.e. from the point (x_n, y_n) to the point $(x_n + h, y_{n+1})$. The increment is defined by the incremental function Φ:

$$y_{n+1} = y_n + \Phi(F; x_n, h; y_n, y_{n+1});$$

with a step size h. This is an implicit method. If Φ does not depend on y_{n+1}, we have an explicit method.

Whatever the choice of Φ, for an implicit method we will need, in general, to solve a non-linear equation ($\rightarrow$ see lecture on root finding). That means that an implicit method is computationally more expensive than a similar explicit method.

Explicit Single Step Methods: Euler Method

First order ODE

$$y' = f(x, y) \qquad\qquad y_{n+1} = y_n + \Phi(f; x_n, h; y_n)$$

Standard procedure for an unknown function: Taylor expand!

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(x_n) + O(h^3)$$

Keeping only terms of order h, and substituting $y'(x_n) = f(x_n = x_0 + n \cdot h, y_n)$ we obtain

Euler method

$$y_{n+1} = y_n + \underbrace{h\, f(x_n, y_n)}_{=\Phi_{\text{Euler}}(f; x_n, h; y_n)}$$

Local Truncation Error for Euler Method

The local trunction error (LTE) is introduced as:

$$y(x_0 + h) - y_0 \equiv \text{LTE} = \frac{h^2}{2} y''(x_0) + O(h^3)$$

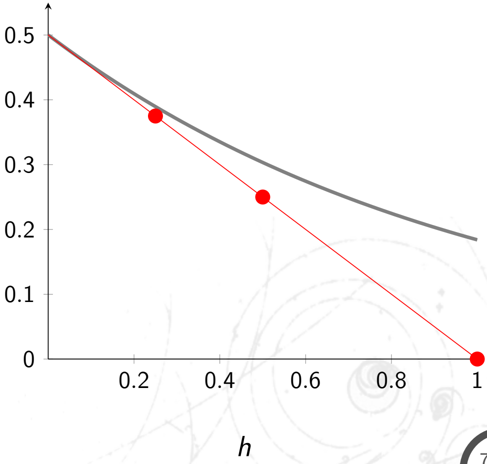
Example

The ODE at hand reads:

$$y' = -y\,, \qquad y_0 = 0.5$$

The analytic solution is:

$$y(x) = y_0 \exp(-x)$$



Explicit Single Step Methods: Runge-Kutta Methods

For Runge-Kutta methods an alternative derivation for the determination y_{n+1} uses an integral representation:

$$y_{n+1} = y_n + \int_{x_n}^{x_n+h} \mathrm{d}x\, f(x, y(x))\,.$$

The s-stage Runge-Kutta method then estimates this integral

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i$$

where

$$\begin{aligned}
k_1 &= f(x_n, & &y_n &)\\
k_2 &= f(x_n + c_2 h, & &y_n + h\, a_{2,1} k_1 &)\\
k_3 &= f(x_n + c_3 h, & &y_n + h\, a_{3,1} k_1 + h\, a_{3,2} k_2 &)\\
&\ \vdots & &\ \vdots & \\
k_s &= (f x_n + c_s h, & &y_n + h\, a_{s,1} k_1 + \cdots + h\, a_{s,(s-1)} k_{s-1} &)
\end{aligned}$$

Now to determine the coefficients $\{a_{i,j}\}$, $\{b_i\}$, and $\{c_i\}$.

Explicit Single Step Methods: Runge-Kutta (cont'd)

Usual presentation of the necessary coefficients in a Butcher tableau:

$$\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{2,1} & & & & \\
c_3 & a_{3,1} & a_{3,2} & & & \\
\vdots & \vdots & & \ddots & & \\
c_s & a_{s,1} & a_{s,2} & \dots & a_{s,s-1} & \\
\hline
 & b_1 & b_2 & \dots & b_{s-1} & b_s
\end{array}$$

To take away:

- a method of stage s requires in general s evaluations of f
- the LTE is of order p, i.e.: $\text{LTE} = O(h^{p+1})$
- in general $s > p$
- up to $s = 4$ there are methods known with $s \geq p$

Explicit Single Step Methods: Runge-Kutta (cont'd)

Euler's method

$$\begin{array}{c|c} 0 & \\ \hline & b_1 \end{array}$$

- method of stage 1 and order 1

Ralston's method

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

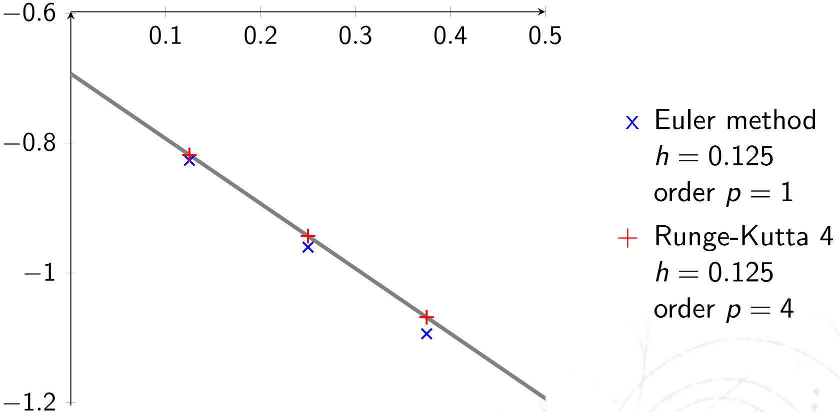
- method of stage 2 and order 2

RK4 (*The* Runge-Kutta method)

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

- method of stage 4 and order 4

Global Truncation Error/Accumulated Error



The differences in accumulated trunction errors is clearly visible

Wastefulness of Single-Step Methods

In order to achieve a single step, the previously shown methods of stage s evaluate the function $f(x; y)$ in at least s points.

However, all the information obtained from these evaluations is thrown away before the next step.

It would be efficient to reuse this information, which gives rise to the multiple step methods.

Multiple Step Methods

An explicit multiple step method of length m follows from:

$$y_{n+1} = -\sum_{j=0}^{m-1} a_j\, y_{n-j} + h \sum_{j=0}^{m-1} b_j\, f(x_{n-j}, y_{n-j})$$

Again, one strives to choose the coefficients $\{a_i\}$ and $\{b_i\}$ such that the LTE is of high order in h.

Adams-Bashforth methods

In Adams-Bashforth methods one chooses $a_0 = -1$, and $a_i = 0$ for $i \geq 1$. The coefficients $\{b_i\}$ are chosen such that $y(x)$ is interpolated in the last m steps:

$$b_{m-j-1} = \frac{(-1)^j}{j!\,(m-j-1)!} \int_0^1 \prod_{i=0, i\neq j}^{s-1} \mathrm{d}u\,(u+i)\,.$$

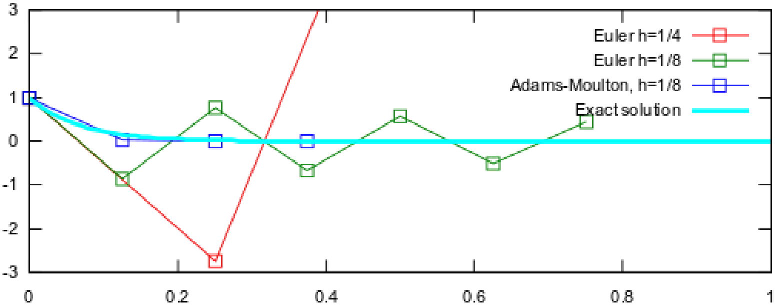
for $j = 0, \ldots, m-1$.

The order p of any Adams-Bashforth method is $p = m$.

Stiff ODEs

Example ODE

$$y' = -15\,y \qquad \text{with} \quad y(x_0) = y_0 = 1.0\,.$$



shamelessly taken from Wikipedia

Stiff ODEs

Example ODE

$$y' = -15\,y \qquad \text{with} \quad y(x_0) = y_0 = 1.0\,.$$

- a stiff ODE forces you to go to unreasonably small step size h in order to have reasonable convergence of the method
- in general, explicit methods demand smaller step sizes than computationally reasonable
- implicit methods solve this problem at the expense of additional evaluations of the generation function F when solving for the increment

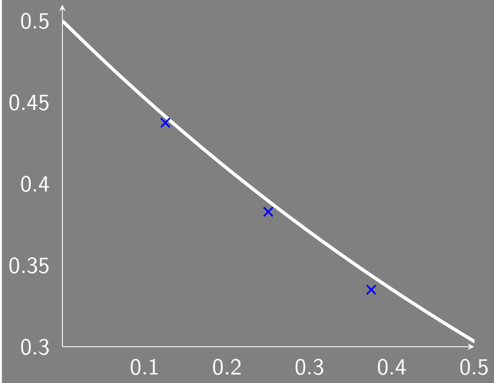
Implicit Euler Method

(Also known as the backward Euler method)

$$y_{n+1} = y_n + h \cdot f(x_{n+1}, y_{n+1})$$

Example with stiff ODE

$$y' = -y, \qquad \text{with} \quad y_0 = y(x_0) = 0.5$$



× regular Euler
$h = 0.125$

Implicit Euler Method

(Also known as the backward Euler method)

$$y_{n+1} = y_n + h \cdot f(x_{n+1}, y_{n+1})$$

Example with stiff ODE

$$y' = -y, \qquad \text{with} \quad y_0 = y(x_0) = 0.5$$

$$\begin{aligned} y_{n+1} &= y_n + h\, f(x_{n+1}, y_{n+1}) \\ &= y_n - h\, y_{n+1} \\ \Rightarrow y_{n+1} &= \frac{y_n}{1+h} \end{aligned}$$

This yields the analytic result in the limit $h \to 0$ ($h = h_0/n$, $n \to \infty$), since:

$$\lim_{n\to\infty} \frac{y_0}{(1+\frac{x}{n})^n} = y_0 \exp(-x)$$

Implicit Euler Method

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Example with stiff ODE

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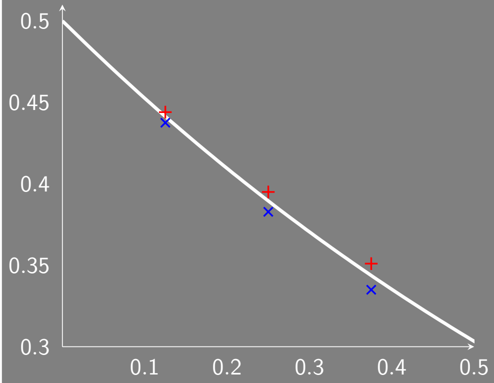

× regular Euler $h = 0.125$

+ implicit Euler $h = 0.125$

Next time on Ordinary Differential Equations

- implicit Runge-Kutta methods

- how to turn an n-order ODE into an n-size system of first-order ODEs

- a glimpse at boundary problems

Backup