Numerical Methods in Physics

Numerische Methoden in der Physik, 515.421.

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Room: TDK Seminarraum

Time: 8:30-10 a.m.

Exercises: Computer Room, PH EG 004 F

http://itp.tugraz.at/LV/boeri/NUM_METH/index.html
(Lecture slides, Script, Exercises, etc).

Last week(26/11/2013)

Numerical Solution of Transcendental Equations:

- Gross search for the zeroes of a function.
- The Newton-Raphson method: a program.
- Other methods for finding zeroes of a function: False position (*regula falsi*).
- **Bisection** method (nested intervals).

Zeroes of a Trascendental Equation: Summary

$$F(x) = 0$$

The values of *x* which satisfy this equation are called **zeroes**, **solutions** or **roots** of the function.

$$f(x) = x$$

We have considered the special case in which the transcendental equation can be solved for x.

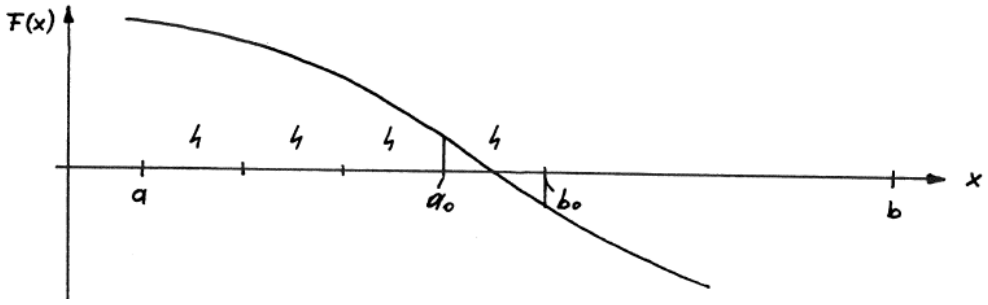
We considered **two classes** of methods:

- **Iterative methods:** Newton-Raphson (tangent) and Regula Falsi - false position (secant).
- Method of the nested intervals (**bisection**).

Both classes of methods permit to find the zeroes of a function in a given interval. To use them in practice, they have to be combined with a preliminary gross search for zeroes on the large interval, in which the solution are sought.

Gross Search:

The Newton-Raphson (and the bisection) method permit to find a zero **in a given interval**, **once we know there is a zero**.



In practice, before using any methods to find zeroes, one always performs first a **gross search.**

1) Choose a large interval [a,b].

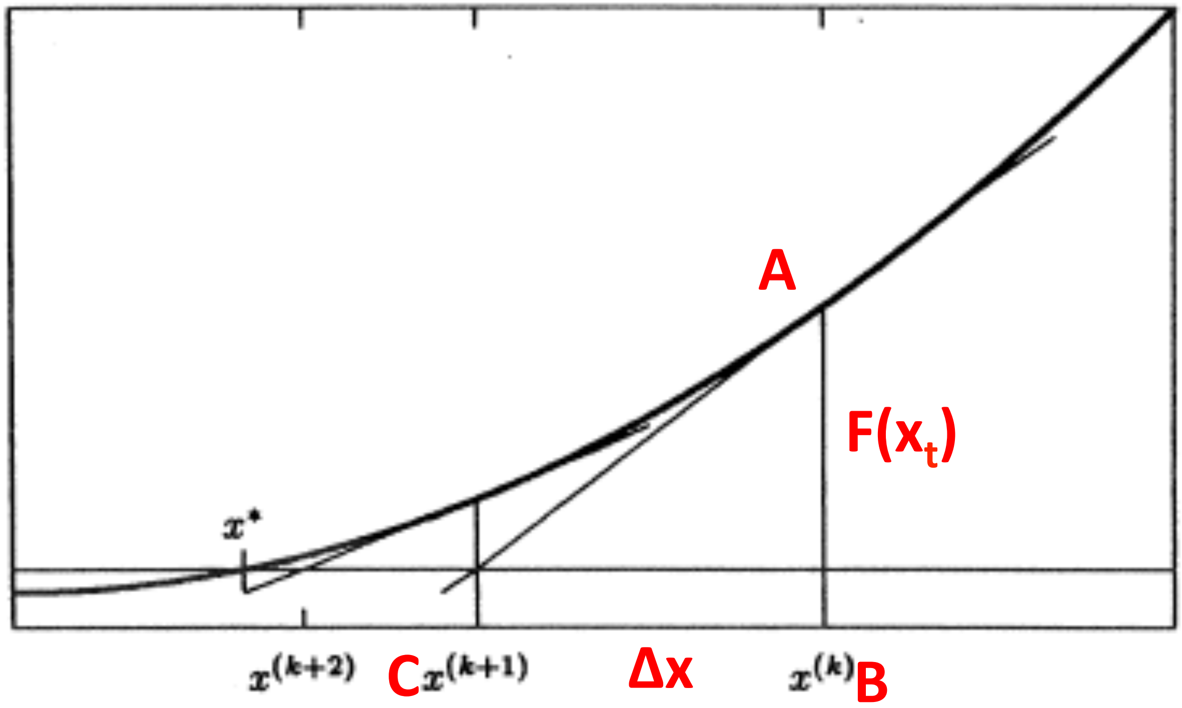
2) Divide it into *n* intervals of width h (stepsize).

3) Compute $s=f(x_{min})xf(x_{max})$ for every interval.

4) If $s \leq 0$, the interval contains a zero, which can be located with a N-R or bissection method.

Newton-Raphson (tangent) method:

$$x_{t+1} = x_t - \frac{F(x_t)}{F'(x_t)}$$



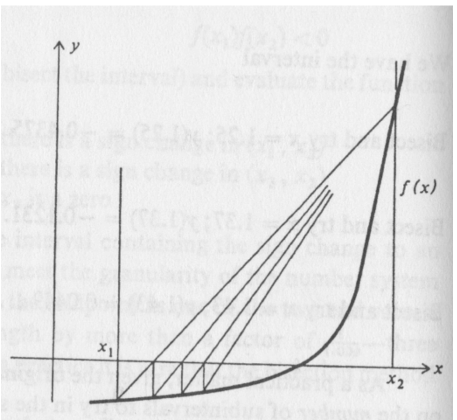
$$\frac{AB}{BC} = F'(x_t)$$

$$\frac{f(x_t)}{\Delta x_t} = F'(x_t) \Rightarrow \Delta x_t = \frac{F(x_t)}{F'(x_t)}$$

False position (*regula falsi*).

It is used to find the zero of a function in an interval [*a*,*b*], **in which the function changes sign**.

The real curve - F(x) - is replaced by the straight line through the two extrema of the interval.



The line between *a* and *b* is given by: $y(x) = \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$

And the zero is: $\overline{x} = a - f(a)\frac{(b - a)}{f(b) - f(a)} = \frac{af(b) - bf(a)}{f(b) - f(a)}$

$$x_{t+1} = x_t - \frac{f(x_t)}{f(x_t) - f(x_{t-1})}(x_t - x_{t-1})$$

Disadvantages: the zero is approached by one side -> The method may be very slow-> ***modified r.f!***

The bissection method (nested intervals):

Given an interval x_1, x_2 in which the function F(x) changes sign – $f(x_1)f(x_2)<0$:

1) The interval is divided in half, picking the midpoint x_3

2) Evaluate the product $f(x_1)f(x_3)$

$$f(x_1)f(x_3)\begin{cases} <0 \text{ the zero is in } x_1, x_3 \\ >0 \text{ the zero is in } x_2, x_3 \\ =0 \text{ the zero is } x_3 \end{cases}$$

3) Iterate the method using the new interval, until the zero is found.

! *h* limits the resolution of the bisection method! Two zeroes can be discriminated only if their distance is larger than h_{res}!

TOPICS (this year):

- **Chapter 1: Introduction.** ✖
- **Chapter 2: Numerical methods for the solution of linear inhomogeneous systems.** ✖
- Chapter 3: Interpolation of point sets.
- **Chapter 4: Least-Squares Approximation.** ✖
- **Chapter 5: Numerical solution of transcendental equations.** ✖
- Chapter 6: Numerical Integration.
- Chapter 7: Eigenvalues and Eigenvectors of real matrices.
- **Chapter 8: Numerical Methods for the solution of ordinary differential equations: initial value problems.**
- Chapter 9: Numerical Methods for the solution of ordinary differential equations: marginal value problems.

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- **Chapter 7: Eigenvalues and Eigenvectors of real matrices.** NEXT
- **Chapter 8: Numerical Methods for the solution of ordinary differential equations: initial value problems.**
- Chapter 9: Numerical Methods for the solution of ordinary differential equations: marginal value problems.

This week(3/12/2013)

Ordinary Differential Equations: Initial Value problems

- Initial Value problems: Definitions.
- Reduction of an n^{th}-order differential equation to a system of N first-order equations.
- Solution of a first-order differential system of equations: Runge-Kutta methods.
- Simple, modified and improved Euler's methods.
- Fourth-order Runge-Kutta formulas: classical Runge Kutta formula, meaning and examples.

Numerical Methods for the solution of ordinary differential equations: initial value problems.

Definition: A differential equation is a mathematical equation for an unknown function of one or several variables that relates the values of the function itself and its derivatives of various orders.

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

Explicit differential equations are those which can be solved for the highest possible derivative *n*:

$$y^{(n)} = F(x; y, y', .., y^{(n-1)})$$

n (i.e. the order of the highest possible derivative) is called the order of a differential equation (or system of equations, if ***x***, ***y***, ***F*** are vectors). **y**(x) is the *solution* of the differential equation.

Differential equations of n^{th} order can be recast into a set of 1^{st} order differential equations, through the following substitution:

$$y^{(n)} = F(x; y, y', .., y^{(n-1)})$$

$$y'_1 = y_2 \equiv f_1(x)$$
$$y'_2 = y_3 \equiv f_2(x)$$
$$\ldots$$
$$y'_{n-1} = y_n = f_{n-1}(x)$$
$$y'_n = F(x; y_1, y_2, .., y_n) = f_n(x)$$

In compact (vector) notation:

$$\mathbf{y}' = f(x, \mathbf{y})$$

Numerical Methods for differential equations do not return the most general solution (function + integration constants), but only permit to calculate the solution on a specific set of points. However, they permit to calculate the solution also in many cases in which the analytical solution is not known (or not possible).

Boundary conditions: In order for a differential problem to be solved numerically, we have to specify the analytical relation between the function and its derivative, as well as the conditions that the solution has to obey in particular points of space.

Initial value problems: In this case, we know the values that solution and its derivatives in a given point x_0. In compact form, the differential system is given by:

$$\mathbf{y}' = f(x, \mathbf{y}) \qquad \text{with } \mathbf{y}(x_0) = \mathbf{y}_0$$

Taylor expansion of the solution:

We assume that we can expand the solution in Taylor series (p-th order) around the point (**$\mathbf{x}_0,\mathbf{y}_0$**):

$$y_i(x) = \sum_{\nu=0}^{p} \frac{(x-x_0)^\nu}{\nu!}\left[\frac{d^\nu}{dx^\nu} y_i(x)\right]_{x_0,\mathbf{y}_0} + R_i(x)$$

If the solution is "well behaved" there is an upper value to the error (*Lagrange residual*):

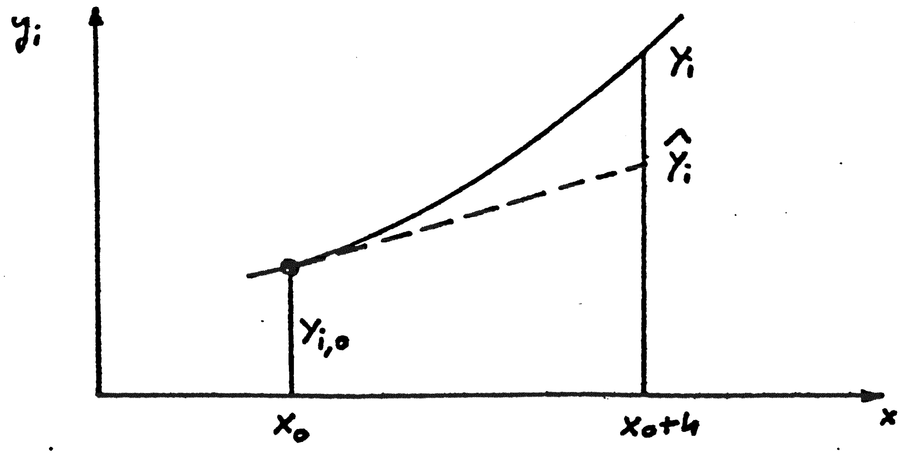
$$R_i(x) = \frac{(x-x_0)^{p+1}}{(p+1)!}\left[\frac{d^{p+1}}{dx^{p+1}} y_i(x)\right]_{x=\xi}, \quad x_0 \le \xi \le x$$

We can then use the Taylor formula to estimate the value of the solution in the point **$\mathbf{x}_0$**+h:

$$\hat{y}_i(x_0+h) = \sum_{\nu=0}^{p} \frac{h^\nu}{\nu!}\left[\frac{d^\nu}{dx^\nu} y_i(x)\right]_{x_0,\mathbf{y}_0}$$

Euler's method: The most ancient method to approximate the solution is the first-order Euler's method; the value of the function is approximated by its tangent times the length of the interval.

$$\hat{y}_i(x_0+h) = y_i(x_0) + h\cdot y'(x)\Big|_{x=x_0} = y_i(x_0) + h\cdot f_i(x_0,\mathbf{y}_0)$$



Leonhard Euler (1707-1783)

Runge-Kutta Methods:

Runge-Kutta methods are among the most popular methods for initial value problems. They are used alone, or as "pre-condition" methods for more refined algorithms (predictor-corrector methods). The biggest ***disadvantage*** is that it is difficult to obtain a reliable error estimate.

Properties:

- **Runge-Kutta** methods derive from a Taylor series expansion of the solution, truncated at p order. P is the **order of the R-K method**.

- Runge-Kutta methods are ***one-step*** methods: in order to determine the value of the solution in $\mathbf{x_0+h}$, it is enough to know its value in the previous point x_0.

- In order to calculate the approximate value of $\mathbf{y(x)}$, it's enough to know $\mathbf{f(x_0,y_0)}$, but not its derivatives!

Runge-Kutta *Ansatz (2nd order)*:

$$\hat{y}(x_0 + h) = y_0 + h \cdot (c_1 g_1 + c_2 g_2)$$

with

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + a_2 h, y_0 + b_{2,1} h g_1)$$

The *Runge-Kutta* coefficients satisfy the following conditions:

$$c_1 + c_2 = 1$$

$$c_2 \cdot a_2 = \frac{1}{2}$$

$$c_2 \cdot b_{2,1} = \frac{1}{2}$$

There are three equations for four coefficients: the system is underdetermined, *i.e.* there is an infinite set of solutions for this system of equations.

The **proof** begins with a *Taylor expansion* of the solution:

RUNGE-KUTTA (RK1)

$$\boxed{\hat{y}(x_0+h) = y_0 + h\,(c_1 g_1 + c_2 g_2)}$$

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + a_2 h,\; y_0 + b_{2,1}\, h\, g_1)$$

TAYLOR (II^nd order)

$$\boxed{y(x_0,h) = y_0 + h\cdot y'(x)\big|_{x=x_0} + \frac{h^2}{2}\, y''(x)\big|_{x=x_0}} = y_0 + h\cdot f(x_0,y_0) + \frac{h^2}{2}\frac{d}{dx}\left[f(x, y(x))\right]\Big|_{x=x_0,\, y=y_0} =$$

$$= y_0 + h\cdot f(x_0,y_0) + \frac{h^2}{2}\left[f_x(x_0,y_0) + f_y(x_0,y_0)\cdot y'(x)\right]\Big|_{(x_0,y_0)} =$$

$$= y_0 + h\, f(x_0,y_0) + \frac{h^2}{2}\left[f_x(x_0,y_0) + f_y(x_0,y_0)\cdot f(x_0,y_0)\right] = y_{TAYLOR}\ (2^{nd}\text{ order})$$

$$g_2 = g_2(h=0) + h\cdot g_2'(h)\big|_{h=0} + \frac{h^2}{2}\, g''(h)\big|_{h=0} = f(x_0,y_0) + h\cdot\left[a_2 f_x(x_0,y_0) + \right.$$

$$\left. + b_{2,1}\, g_1 \cdot f_y(x_0,y_0)\right] + o(h^2) = f(x_0,y_0) + a_2 h\, f_x(x_0,y_0) + b_{2,1} h\, f_y(x_0,y_0)\, f(x_0,y_0) =$$

RK2

$\Rightarrow$

$$\hat{y}(x_0, h) = y_0 + h f(x_0, y_0) \cdot c_1 + c_2 h f(x_0, y_0) + c_2 a_2 h^2 f_x(x_0, y_0) + c_2 b_{2,1} h^2 \cdot f_y(x_0, y_0) \cdot f(x_0, y_0) = y_{TAYLOR}^{2nd}$$

$\Rightarrow$ Order 1 coefficients:

$$f(x_0, y_0)[c_1 h + c_2 h] = f(x_0, y_0) \cdot h [c_1 + c_2] = h \cdot f(x_0, y_0) \Rightarrow \boxed{c_1 + c_2 = 1} \quad (1)$$

$\Rightarrow$ Order 2 coefficients:

$$h^2 [c_2 a_2 f_x(x_0, y_0) + c_2 b_{2,1} \cdot f_y(x_0, y_0) \cdot f(x_0, y_0)] = \frac{h^2}{2} [f_x(x_0, y_0) + f_y(x_0, y_0) f(x_0, y_0)]$$

$$\boxed{c_2 \cdot a_2 = \frac{1}{2}} \quad (2)$$

$$\boxed{c_2 b_{2,1} = 1} \quad (3)$$

$$c_1 = 0, \quad c_2 = 1, \quad a_2 = \frac{1}{2}, \qquad b_{2,1} = \frac{1}{2}$$

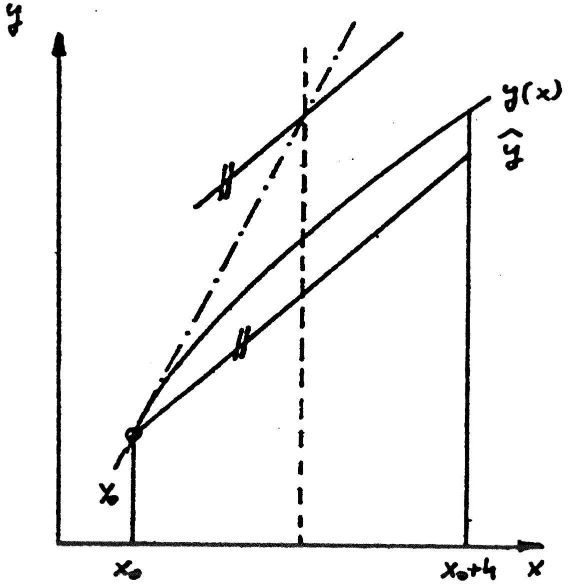
$$\hat{y}(x_0 + h) = y_0 + h \cdot (c_1 g_1 + c_2 g_2)$$

with

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + a_2 h, y_0 + b_{2,1} h g_1)$$

$$\hat{y}(x_0 + h) = y_0 + h \cdot f\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)\right)$$



Modified Euler's method: The solution is approximated by a straight line through ($\mathbf{x}_0, \mathbf{y}_0$) with the slope of *y(x)* in the middle point of the interval $[x_0, x_0+h]$.

$$c_1 = \frac{1}{2}, \quad c_2 = \frac{1}{2}, \quad a_2 = 1, \quad b_{2,1} = 1$$

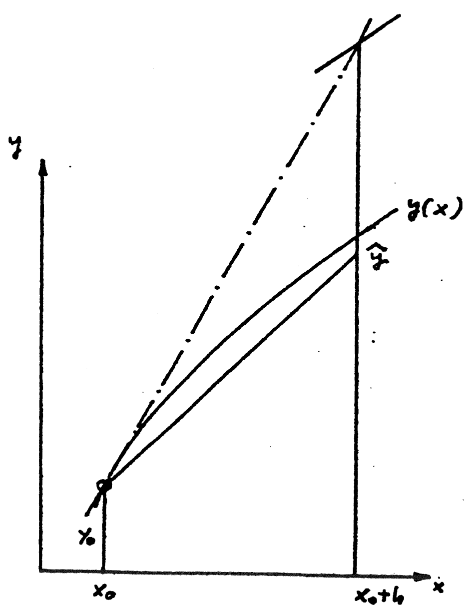
$$\hat{y}(x_0 + h) = y_0 + h \cdot (c_1 g_1 + c_2 g_2)$$

with

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + a_2 h, y_0 + b_{2,1} h g_1)$$

$$\hat{y}(x_0 + h) = y_0 + h \cdot \left\{ \frac{1}{2} f(x_0, y_0) + \frac{1}{2} f\left[x_0 + h, y_0 + hf(x_0, y_0) \right] \right\}$$



Improved Euler's method: The solution is approximated by a straight line through (**x_0**,**y_0**), whose slope is the arithmetic average between $y'(x_0)$ and $y'(x_0+h)$.

Example:

$$y'(x) = f(x) = e^x, \qquad y(0)=0$$

Exact solution: $y(x) = e^x - 1$

What is the approximate value given by the three Runge-Kutta formulas seen so far for *x=1*?

Euler's Method:

$$\hat{y}(x_0 + h) = y(x_0) + h \cdot f(x_0, \mathbf{y}_0)$$

Modified Euler's Method:

$$\hat{y}(x_0 + h) = y_0 + h \cdot f(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0))$$

Improved Euler's Method:

$$\hat{y}(x_0 + h) = y_0 + h \cdot \left\{ \frac{1}{2} f(x_0, y_0) + \frac{1}{2} f\left[x_0 + h, y_0 + hf(x_0, y_0)\right] \right\}$$

Solution:

Runge - kutta, 1st and 2nd order, evaluate $\hat{y}(1)$ for $e^x - 1 = y(x)$ (RK S1)

$f(x, y) = e^x$

$(x_0, y_0) = (0, 0)$

$h = 1$

Euler's formula:

$$\hat{y}(x_0 + h) = y(x_0) + h \cdot f(x_0, y_0) = \emptyset + h \cdot 1 = 1$$

Modified Euler's Method:

$$\hat{y}(x_0 + h) = y(x_0) + h \cdot f\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)\right) = \emptyset + 1 \cdot e^{\frac{1}{2}} = 1.64872$$

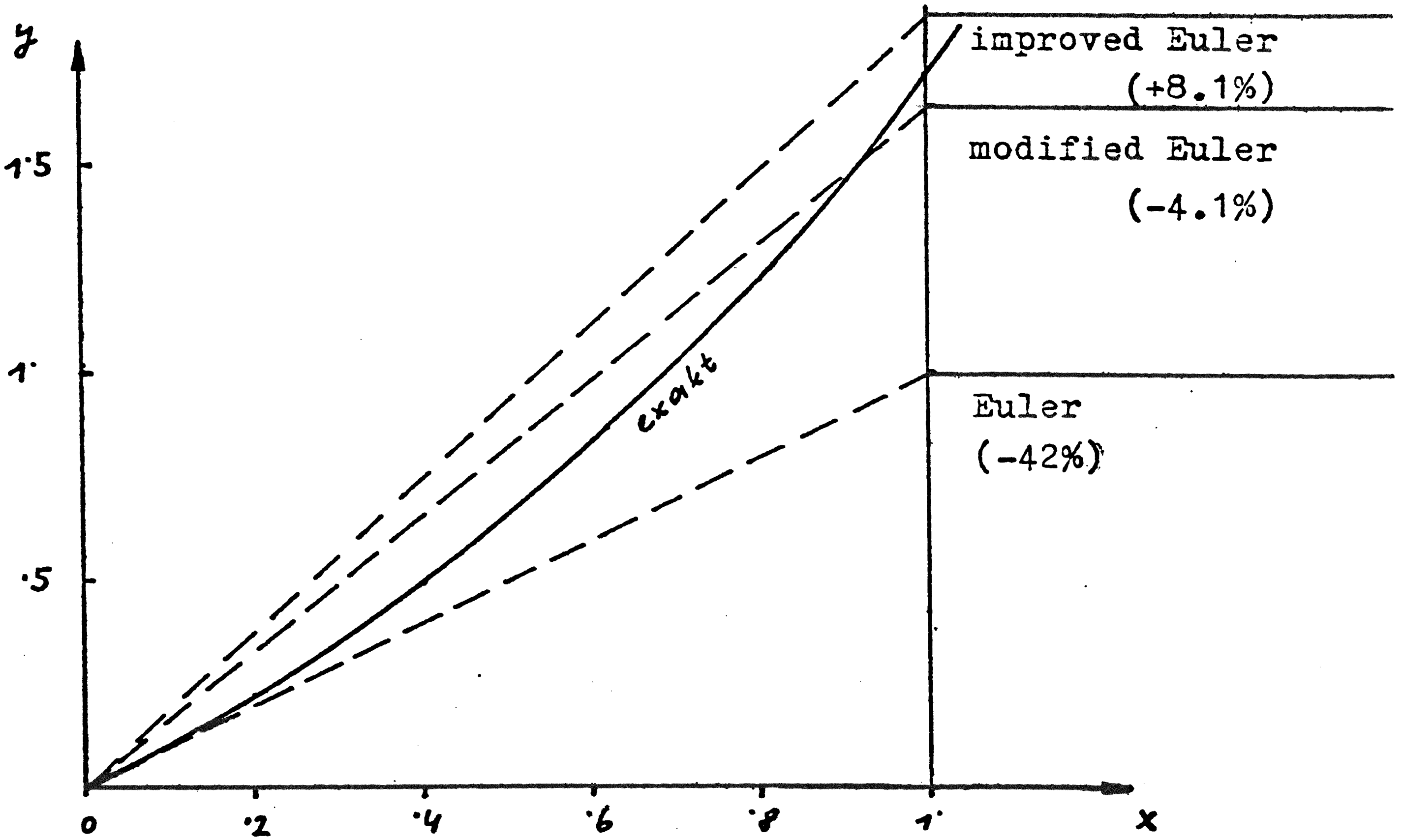
Improved Euler's Method:

$$\hat{y}(x_0 + h) = y_0 + h \left\{ \frac{1}{2} f(x_0, y_0) + \frac{1}{2} f\left[x_0 + h, y_0 + h f(x_0, y_0)\right] \right\} =$$

$$= \emptyset + 1 \left\{ \frac{1}{2} + \frac{f(1)}{2} \right\} = 1.85914091$$

Exact solution $= e^1 - 1 = 1.7182818...$

Error (graphical representation):



Higher order Runge-Kutta Methods:

Runge-Kutta formulas can be derived for arbitrary *p* order. The corresponding *ansatz* is:

$$\hat{y}_i(x_0 + h) = y_i(x_0) + h\sum_{j=1}^{p} c_j g_j$$

$$g_1 = f(x_0, y_0)$$

$$g_j = f(x_0 + a_j h; y_0 + h\sum_{l=1}^{j-1} b_{j,1} g_l)$$

The first g's are for example:

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + a_2 h, y_0 + hb_{2,1} g_1)$$

$$g_3 = f(x_0 + a_3 h, y_0 + hb_{3,2} g_2 + hb_{3,1} g_1)$$

The p-th Runge-Kutta formulas contain 3 types of coefficients ($c_i, a_i, b_{i,j}$), which are mutually related by recursion formulas. The total number of coefficients is $(p^2+3p-2)/2$:

$$c_1,\ldots,c_p \quad p \text{ coefficients}$$

$$a_2,\ldots,a_{p-1} \quad (p-1) \text{ coefficients}$$

$$b_{2,1}\ldots b_{p,p-1} \quad p(p-1)/2 \text{ coefficients}$$

These coefficients are often tabulated in this form:

$$\begin{array}{c|ccccc}
a_2 & b_{2,1} & & & & \\
a_3 & b_{3,1} & b_{3,2} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
a_p & b_{p,1} & b_{p,2} & \cdots & b_{p,p-1} & \\
\hline
 & c_1 & c_2 & \cdots & c_{p-1} & c_p
\end{array}$$

The most used Runge-Kutta methods are *fourth-order* methods.

Classical Runge-Kutta formula:

$1/2$	$1/2$			
$1/2$	0	$1/2$		
1	0	0	1	
	$1/6$	$1/3$	$1/3$	$1/6$

a_2	$b_{2,1}$				
a_3	$b_{3,1}$	$b_{3,2}$			
$\vdots$	$\vdots$	$\vdots$	$\ddots$		
a_p	$b_{p,1}$	$b_{p,2}$	$\dots$	$b_{p,p-1}$	
	c_1	c_2	$\dots$	c_{p-1}	c_p

3/8 Runge-Kutta formula:

$1/3$	$1/3$			
$2/3$	$-1/3$	1		
1	1	-1	1	
	$1/8$	$3/8$	$3/8$	$1/8$

Classical Runge-Kutta formula:

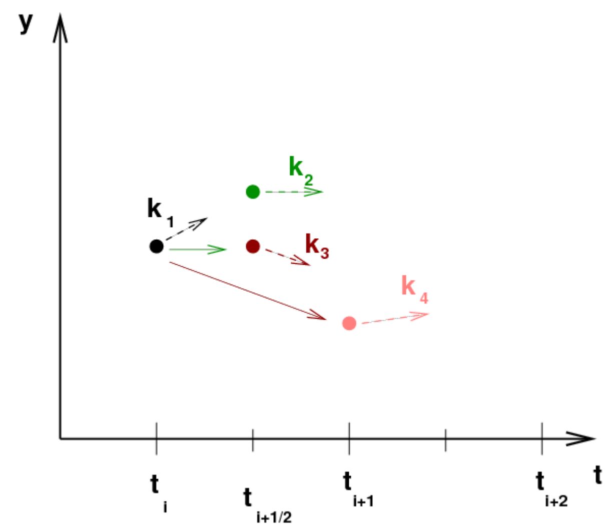
$$\hat{y}(x_0 + h) = y(x_0) + h\left[\frac{1}{6}g_1 + \frac{1}{3}g_2 + \frac{1}{3}g_3 + \frac{1}{6}g_4\right]$$

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + \frac{h}{2}; y_0 + \frac{h}{2}g_1)$$

$$g_3 = f(x_0 + \frac{h}{2}, y_0 + \frac{h}{2}g_2)$$

$$g_4 = f(x_0 + \frac{h}{2}, y_0 + hg_3)$$



Meaning: We start from point $P_0=x_0,y_{0;}$ we use (g_1) the slope of the solution, to make a step forward of size h/2 -> $P_1=(x_1,y_1)=(x_0+h/2,y_0+h/2)$. We use the slope evaluated in $P_1=g_2$ to make another step forward (*h/2*) starting from (x_0,y_0) -> P_2. The new slope is $f(x_0+h/2, y_0+h/2\ g_2)=g_3$. We start again from ($x_0$,$y_0$) and make one final **full** (=h) step forward -> P_3. The “real” slope of the solution is approximated by a weighted average of the slopes in P_0,P_1,P_2,P_3.

For our "old" example:

$$y'(x) = f(x) = e^x, \qquad y(0)=0$$

We have:

$$g_1 = f(x_0, y_0)$$

$$g_2 = f(x_0 + \frac{h}{2}; y_0 + \frac{h}{2} g_1)$$

$$g_3 = f(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} g_2)$$

$$g_4 = f(x_0 + \frac{h}{2}, y_0 + h g_3)$$

$$e = 2.7182818\ldots$$

$$e^{1/2} = 1.64872$$

$$\hat{y}_{RK}(1) = \frac{1}{6} f(0) + \frac{2}{3} f(1/2) + \frac{1}{6} f(1) = 1.7188\ldots$$

$$\left| y(1) - \hat{y}_{RK}(1) \right| \leq 0.0005\ldots$$

Fourth order methods are much more accurate than first and second order methods!

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- Fourth-order Runge-Kutta formulas: classical Runge Kutta formula, meaning and examples.