I3344
Numerical Simulation & Modeling

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Tentative Syllabus

- ✓ Interpolation and extrapolation
  - ✓ Linear: linear regression y = ax + b; correlation, standard deviation, etc.
  - ✓ Non-linear: k nearest neighbors (KNN)
  - ✓ Validation of two models: k-fold cross validation method.
- ✓ Solving a linear equation
  - ✓ Direct methods: Gauss and LU
  - ✓ Iterative methods: Jacobi and Gauss-Seidel
- **Derivation**
  - **Finite difference method (FDM): Euler and Runge-kutta**
- Integration: surface estimation
  - Monte Carlo method.
  - Finite Element Method (FEM).
  - Comparison of two methods.
- Non-linear problems
  - Bisection method
- Introduction to the notion of parallel computing and underlying algorithms

Outline

- What differential equations are?
- First order differential equations
- Solving first order equations using Euler's method.
- Analysis of Euler's method
- Taylor methods
- Euler's midpoint and Runge-Kutta Methods

What are Differential Equations?

Introduction

- Differential equations is an essential tool in a wide range of applications.
- Many **phenomena** can be modeled by a relationship between a function and its derivatives

Examples from Physics

- Consider an object moving through space.
- At time t = 0 it is located at a point P
- After a time t, its distance to P corresponds to f(t)
- Average speed [t, t + Δt]: $f(t + \Delta t) - f(t) / \Delta t$
- Speed at time t : $v(t) = \lim_{\Delta t \to 0} \frac{f(t+\Delta t) - f(t)}{\Delta t}$
- Average acceleration [t, t + Δt]: $v(t + \Delta t) - v(t) / \Delta t$
- Acceleration at time t: $a(t) = \lim_{\Delta t \to 0} \frac{v(t+\Delta t) - v(t)}{\Delta t}$

$$\boxed{v(t) = f'(t), \qquad a(t) = v'(t) = f''(t)}$$

Examples from Physics (cont'd)

- Newton's second law: if an object is influenced by a force, its acceleration is proportional to the force

$$F = ma$$

- Example: object of mass m falling freely towards the earth
  - Influenced by two ***opposite*** forces: gravity and friction
  - Gravitational force: $F_g = mg$
  - Friction: proportional to the v^2: $F_f = cv^2$

$$F = F_g - F_f = ma \Rightarrow mg - cv(t)^2 = mv'(t) \Rightarrow mv' = mg - cv^2$$

General use of differential equations

1. A quantity of interest is modeled by a ***function x***
2. A relation between x and its derivatives is derived from some known principle => ***differential equation*** is obtained
3. The **differential equation** is solved by a ***mathematical*** or ***numerical*** method.
4. The **solution** of the equation is interpreted in the context of the original problem.

Different types of differential equations

- First order differential equation
  - involves the unknown function x and its first derivative x'
- Pth order differential equation
  - involves higher derivatives up to order p
- Linear differential equations

$$x^{(p)}(t)=f(t)+g_0(t)x(t) + g_1(t)x'(t) + g_2(t)x''(t) + \cdots + g_p(t)x^{(p-1)}(t)$$

- Ordinary differential equations
  - Unknown function **depends on <u>only one variable</u>** (denoted by t)
- Partial differential equations
  - Unknown function **depends on <u>two or more variables</u>**
  - Example: three coordinates of a point in space

Exercises

- *Which of the following differential equations are linear?*

a) $x'' + t^2 x' + x = \sin t.$

b) $x''' + (\cos t)x' = x^2.$

c) $x' x = 1.$

d) $x' = 1/(1 + x^2).$

e) $x' = x/(1 + t^2).$

First Order Differential Equations

Introduction

- $x' = f(t, x)$
- $x = x(t)$
- t is the free variable
- Examples of first order differential equations
  - $x' = 3$
  - $x' = 2t$
  - $x' = x$
  - $x' = t^3 + \sqrt{x}$
  - $x' = \sin(tx)$

Scope

Derive **numerical methods** for solving differential equations in the form $x' = f(t, x)$ where f is a given function of two variables

Initial conditions

- **Analytical solutions** of **differential equations** involve a *general constant C* (like indefinite integrals)
- Need to supply an **extra condition** that will specify the value of the constant (called **initial condition**)
- Standard way: specify one point on the solution of the equation => solution should satisfy $x(a) = x_0$ for certain *a*
- Example: $x' = 2x \Rightarrow x = Ce^{2t}\ \forall C$
  - Initial value: $x(0) = 1 \Rightarrow C = 1 \Rightarrow x(t) = e^{2t}$
  - General Initial value: $x(a) = x_0 \Rightarrow x(t) = x_0\, e^{2(t-a)}$
- *Initial condition usually has a concrete physical interpretation*
  - Example: initial speed of a falling object

Definition revisited

"A first order differential equation is an equation in the form $x' = f(t, x)$, where $f(t, x)$ is a function of two variables. In general, this kind of equation has many solutions, but a specific solution is obtained by adding an initial condition $x(a) = x_0$.

A complete formulation of a first order differential equation is:

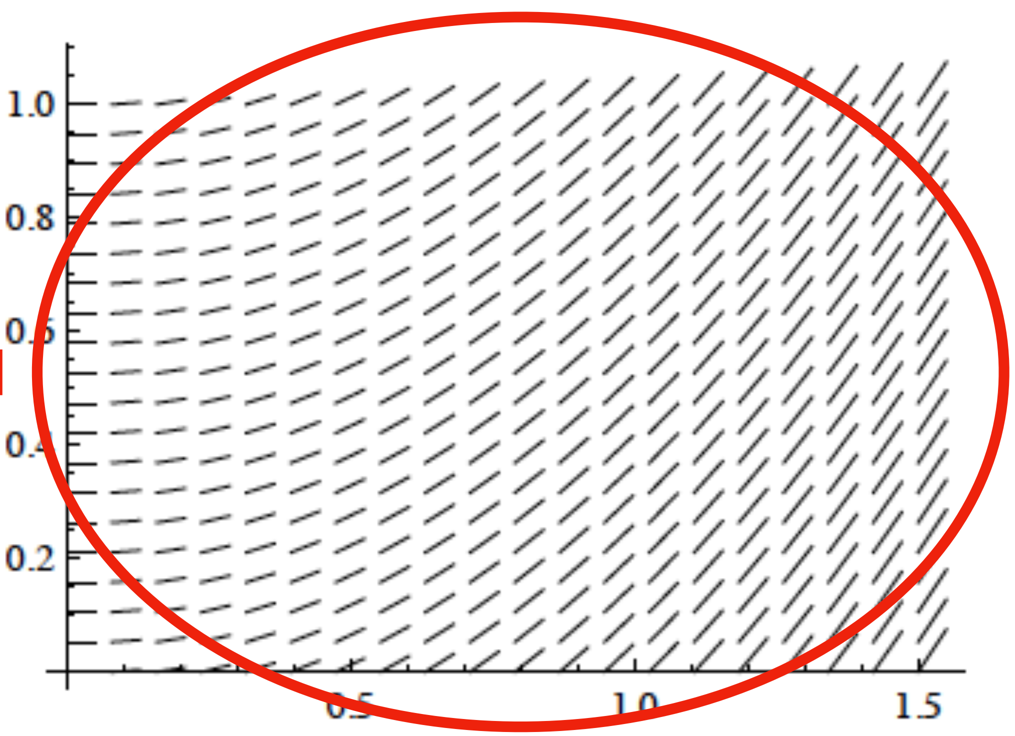
$$x' = f(t, x), \quad x(a) = x_0$$

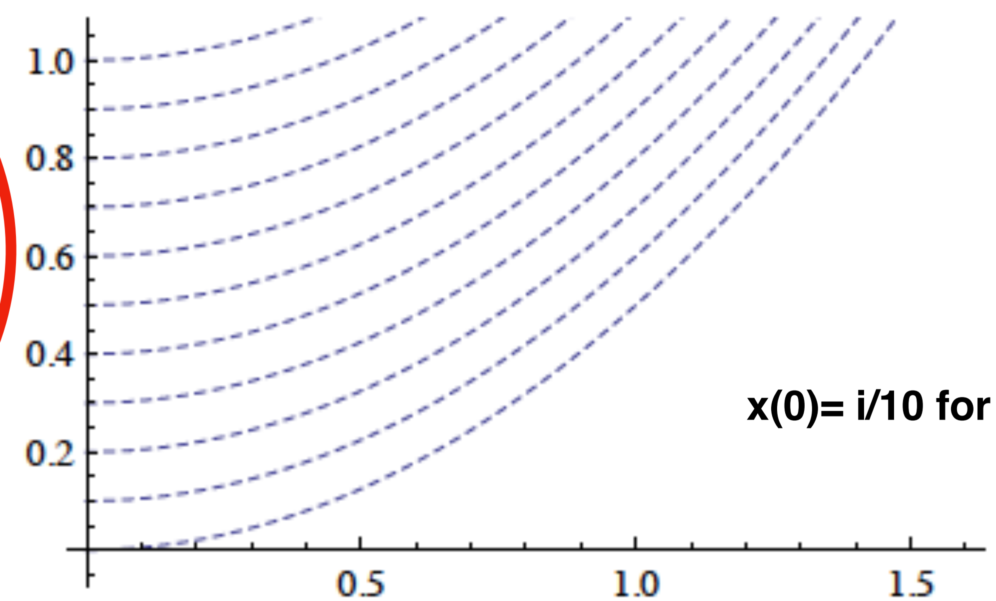
"

Geometric interpretation

- At any point (t, x), the equation x' = f(t, x) prescribes the slope of the solution through this point
- Example: x’= f(t, x) = t
  - This equation describes a family of functions whose tangents have slope t at any point (x,t).

Slope field





x(0)= i/10 for i= 0, 1, . . . , 10

Conditions of existence of one solution

- Example: $x' = \sqrt{1 - x^2}$
  - Condition: $-1 <= x <= +1$
- Main condition: **f(t,x) should no have any problematic behavior**
- Existence and uniqueness

Conditions of existence of one solution

- Exercise: *What features of the following differential equations could cause problems if you try to solve them?*

a) $x' = t/(1-x)$.

b) $x' = x/(1-t)$.

c) $x' = \ln x$.

d) $x'x = 1$.

e) $x' = \arcsin x$.

f) $x' = \sqrt{1-x^2}$.

General strategy for numerical solution of differential equations

- Suppose the differential equation and initial condition: $x' = f(t, x)$, $x(a) = x_0$ are given together, with an interval $[a, b]$ where a solution is sought.
- Suppose also that an increasing sequence of t-values $(t_k)_{k=0...n}$ are given, with $a = t_0$ and $b = t_n$, which in the following will be equally spaced with step length h , i.e., $t_k = a + k.h$, for $k = 0, \ldots, n$.
- A **numerical method for solving the equation** is a recipe for computing a sequence of numbers $x_0, x_1, \ldots, x_n$ such that x_k is an approximation to the true solution $x(t_k)$ at t_k .
- For k > 0, the approximation x_k is computed from one or more of the previous approximations $x_{k-1}, x_{k-2}, \ldots, x_0$.
- Continuous approximation is obtained by **connecting neighboring points by straight lines.**

Euler's method

Introduction

- Methods for **finding analytical solutions** of differential equations often appear rather tricky and unintuitive.
- Many **numerical methods** are based on simple, often **geometric ideas**.
- Euler's Method
  - The simplest of numerical methods
  - Based directly on geometric interpretation of first order differential equation

Basic idea and algorithm

- $x' = f(t, x),\ x(a) = x_0$
- **Aim**: to compute a sequence of approximations $(t_k, x_k)_{k=0..n}$ to the solution where $t_k = a + k.h$
- Initial condition provides a point on the true solution (t_0, x_0)
  - (t_0, x_0) is the natural starting point for the approximation
- To obtain an approximation to the solution at t_1, **compute the slope of the tangent at** (t_0, x_0) as $x'_0 = f(t_0, x_0)$.
- $T_0(t) = x_0 + (t - t_0)\, x'_0$ is the tangent to the solution at t_0 .
- As the approximation x_1 at t_1, use the value of the tangent T_0 which is given by: $x_1 = T_0(t_1) = x_0 + hx'_0 = x_0 + hf(t_0, x_0)$

Basic idea and algorithm (cont'd)

- $x' = f(t, x)$, $x(a) = x_0$, $t_k = a + kh$,
- $T_0(t) = x_0 + (t - t_0)\, x'_0$ is the tangent to the solution at t_0 .
- $x_1 = T_0(t_1) = x_0 + hx'_0 = x_0 + hf(t_0, x_0)$
- **Next step**: find x_2 for t_2
- **How?:** move along the tangent to the exact solution that passes through (t_1, x_1)
- The derivative at this point is $x'_1 = f(t_1, x_1)$
- the tangent at t_1 is : $T_1(t) = x_1 + (t - t_1)x'_1 = x_1 + (t - t_1)\, f(t_1, x_1)$
- The approximate solution at t_2 is: $x_2 = x_1 + h.f(t_1, x_1)$
- $(t_2, x_2) \Rightarrow (t_3, x_3) \Rightarrow \ldots. \Rightarrow (t_n, x_n)$

Basic idea and algorithm (cont'd)

In Euler's method,

an approximate solution (t_k, x_k) *is advanced to* (t_{k+1}, x_{k+1})

by following the ***tangent***

$$\boldsymbol{T_k(t) = x_k + (t - t_k)x'_k = x_k + (t - t_k)\, f(t_k, x_k)} \text{ at } (t_k, x_k)$$

from t_k *to* $t_{k+1} = t_k + h$.

This results in the approximation

$$\boldsymbol{x_{k+1} = x_k + hf(t_k, x_k)} \text{ at } x(t_{k+1})$$

Exercise

- Consider the differential equation: $x' = t^3 - 2x,\ x(0) = 0.25$.
- Suppose we want to compute an approximation to the solution at the points $t_1 = 0.1,\ t_2 = 0.2,\ \ldots,\ t_{10} = 1$, i.e., the points $tk = k*h$ for $k = 1, 2, \ldots, 10$, with $h = 0.1$

Reminder:

In Euler's method, an approximate solution (t_k, x_k) *is advanced to* (t_{k+1}, x_{k+1}) *by following the* ***tangent:***

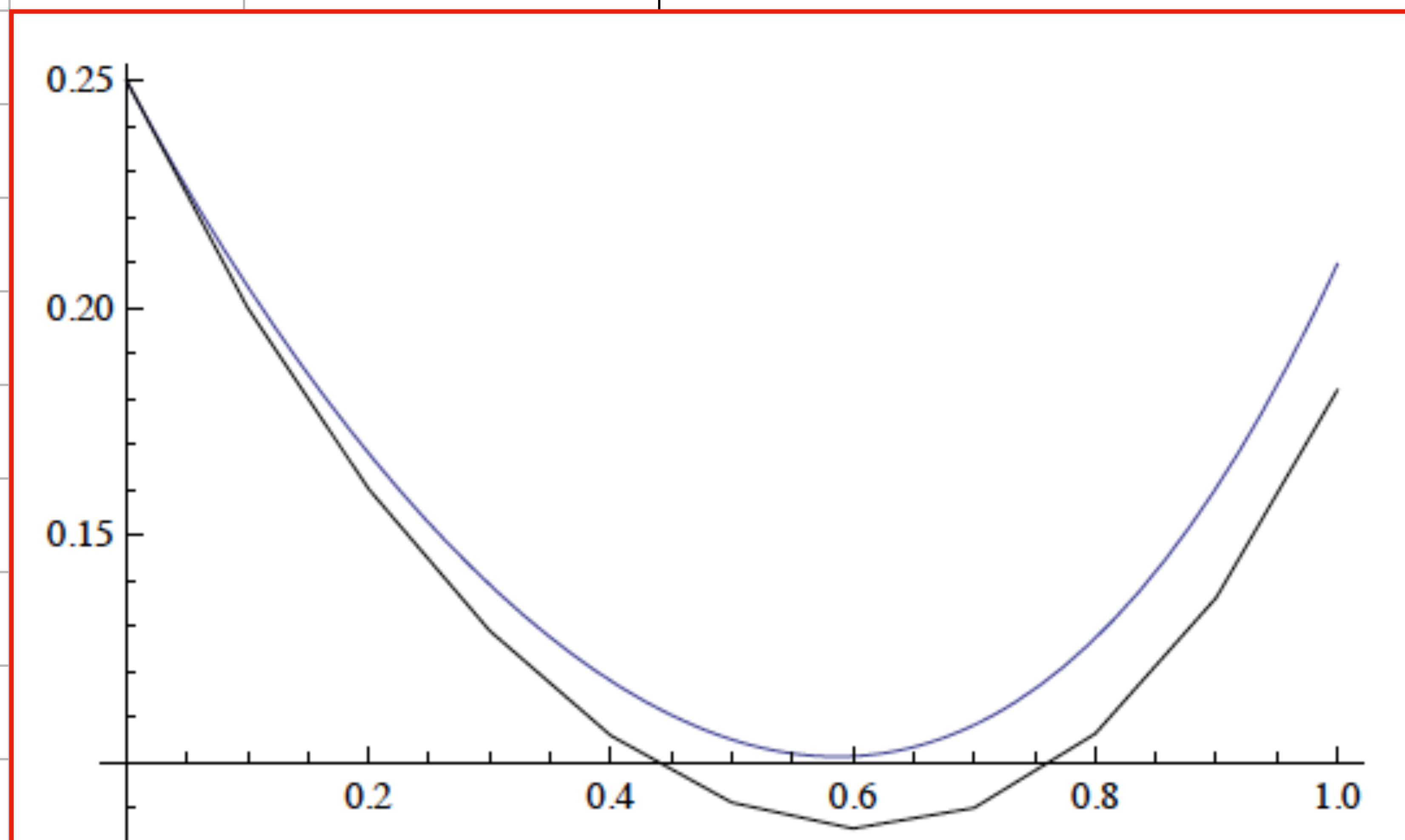
$\mathbf{T_k(t) = x_k + (t - t_k)x'_k = x_k + (t - t_k)\, f(t_k, x_k)}$ *at* (t_k, x_k) *from* t_k *to* $t_{k+1} = t_k + h$.

This results in the approximation: $\mathbf{x_{k+1} = x_k + hf(t_k, x_k)}$ ***at*** $\mathbf{x(t_{k+1})}$

Exercise - Solution

- $x' = t^3 - 2x$

i	t_i	$x(t_i)$	x'_0	$T_i(t)$
0	0	0,25	-0,5	0,25-0,5t
1	0,1	0,2	-0,399	$0{,}2-(t-0{,}1)0{,}399$
2	0,2	0,1601		
3	0,3	0,1289		
4	0,4	0,1058		
5	0,5	0,0910		
6	0,6	0,0853		
7	0,7	0,0899		
8	0,8	0,1062		
9	0,9	0,1362		
10	1	0,1818		



Algorithm

- Let the differential equation $x'=f(t, x)$ be given together with the initial condition $x(a)=x_0$, the solution interval [a, b], and the number of steps n .
- If the following algorithm is performed

$h = (b - a)/n$;

$t_0 = a$;

for $k = 0, 1, . . . , n - 1$

$\quad x_{k+1} = x_k + h f(t_k, x_k)$;

$\quad t_{k+1} = a + (k + 1)h$;

- the value x_k will be an approximation to the solution $x(t_k)$ of the differential equation, for each $k = 0, 1, . . . , n$

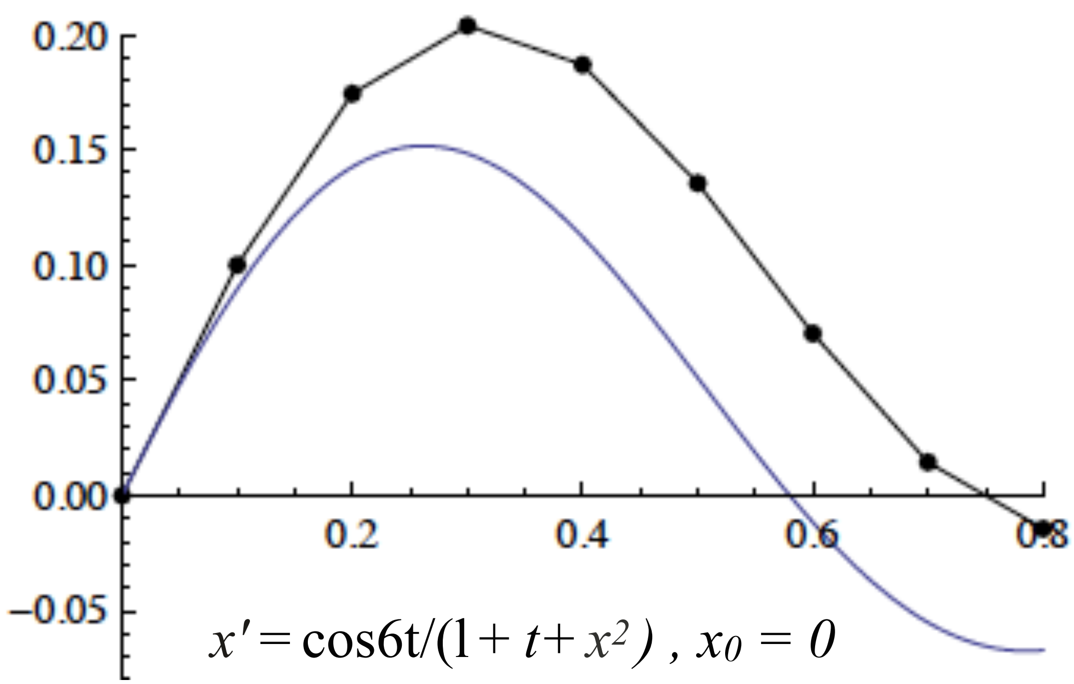
Geometric Interpretation

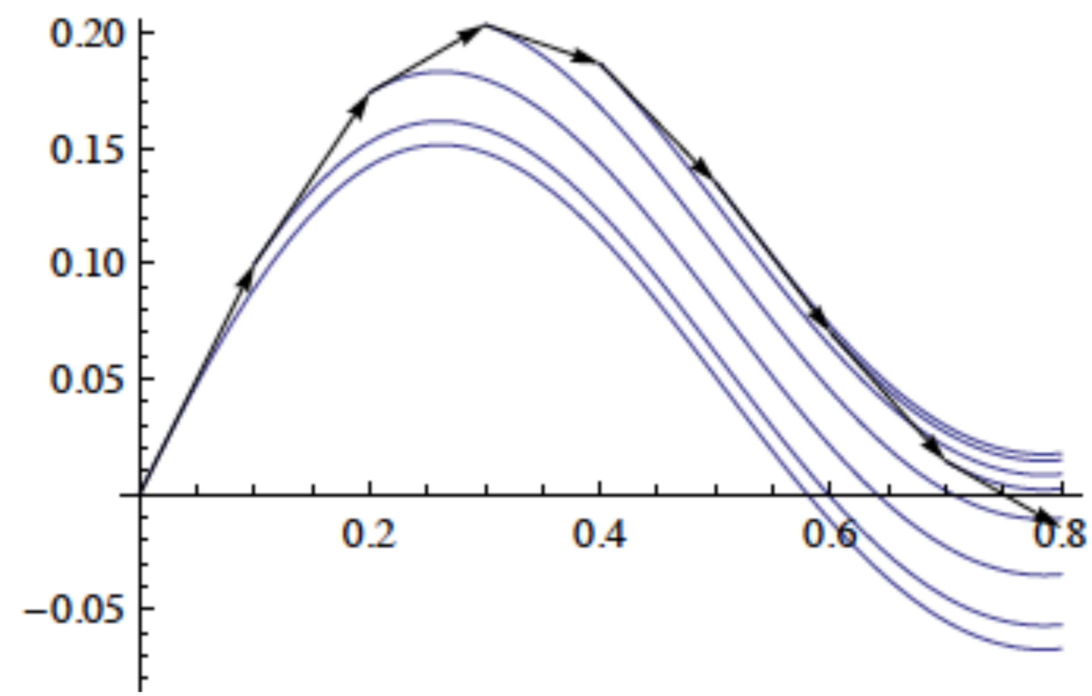
- Euler's method may be interpreted as stepping between different solution curves of the equation x'= f(t,x).
- At time t, the tangent T_k to the solution curve given by

$$x' = f(t, x)\ ,\ x(t_k) = x_k$$

is followed to the point (t_{k+1}, x_{k+1}), which is a point on the solution curve given by

$$x' = f(t, x)\ ,\ x(t_{k+1}) = x_{k+1}$$





Exercises

Use Euler's method with <u>three steps</u> with h = 0.1 to compute approximate solutions of the following differential equations:

a) $x' = t + x, \quad x(0) = 1.$

b) $x' = \cos x, \quad x(0) = 0.$

c) $x' = t/(1 + x^2), \quad x(0) = 1.$

d) $x' = 1/x, \quad x(1) = 1.$

e) $x' = \sqrt{1 - x^2}, \quad x(0) = 0.$

Error analysis for Euler's method

Background

- A function $g(t, x)$ of two variables can be differentiated with respect to t (resp. x) by considering x (resp. t) to be a constant; the resulting derivative is denoted $g'_t(t, x)$ (resp. $g'_x(t, x)$)

- **Taylor polynomial Approximation**: Any function f whose first n + 1 derivatives are continuous at x = a can be expanded in a Taylor polynomial of degree n at x = a with a corresponding error term,

$$f(x) = f(a) + (x-a)f'(a) + \cdots + \frac{(x-a)^n}{n!}f^{(n)}(a) + \frac{(x-a)^{n+1}}{(n+1)!}f^{(n+1)}(\xi_x)$$

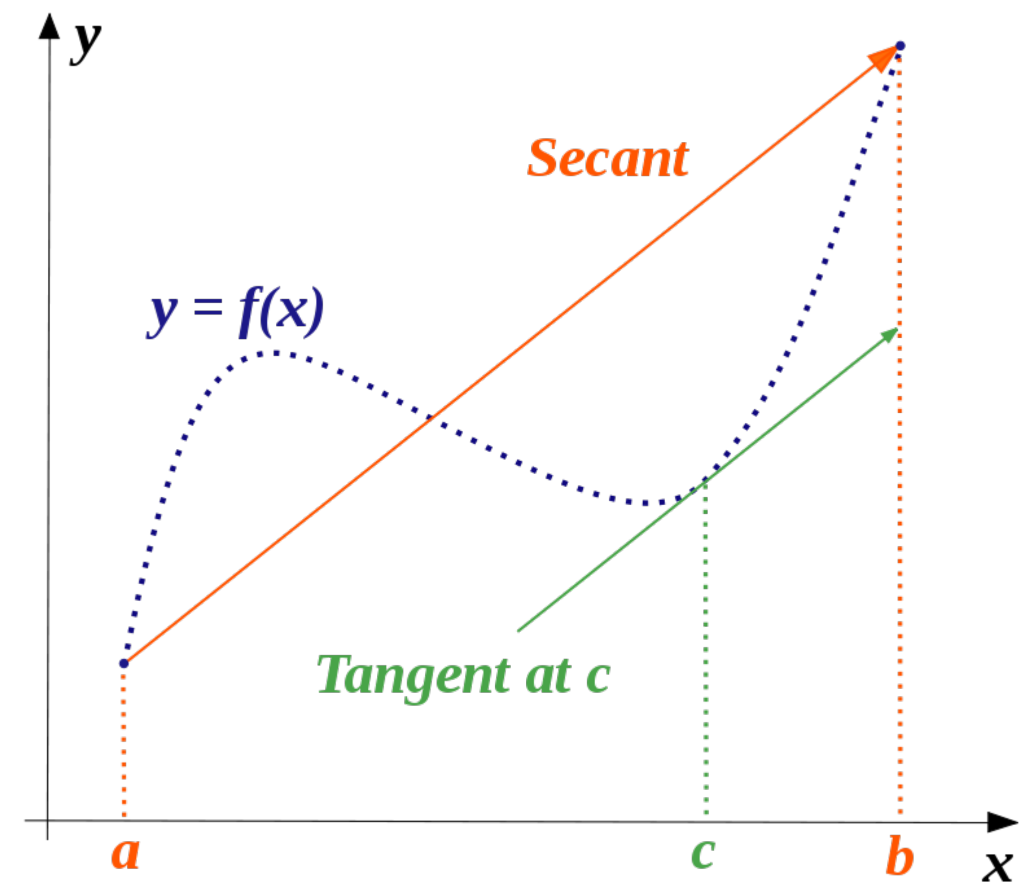
where ξ_x is a number in the interval (a, x) (the interval (x, a) if x < a) that depends on x. This is called a ***Taylor expansion*** of f

Background

- **Mean value theorem**: Let g (t, x) be a function of the two variables t and x, and let g'_x denote the derivative of g with respect to x. If g'_x is continuous in $[x_1,x_2]$ then

$$g(t, x_2) - g(t, x_1) = g'_x(t, \xi)(x_2 - x_1)$$

where ξ is a number in the interval (x_1,x_2)

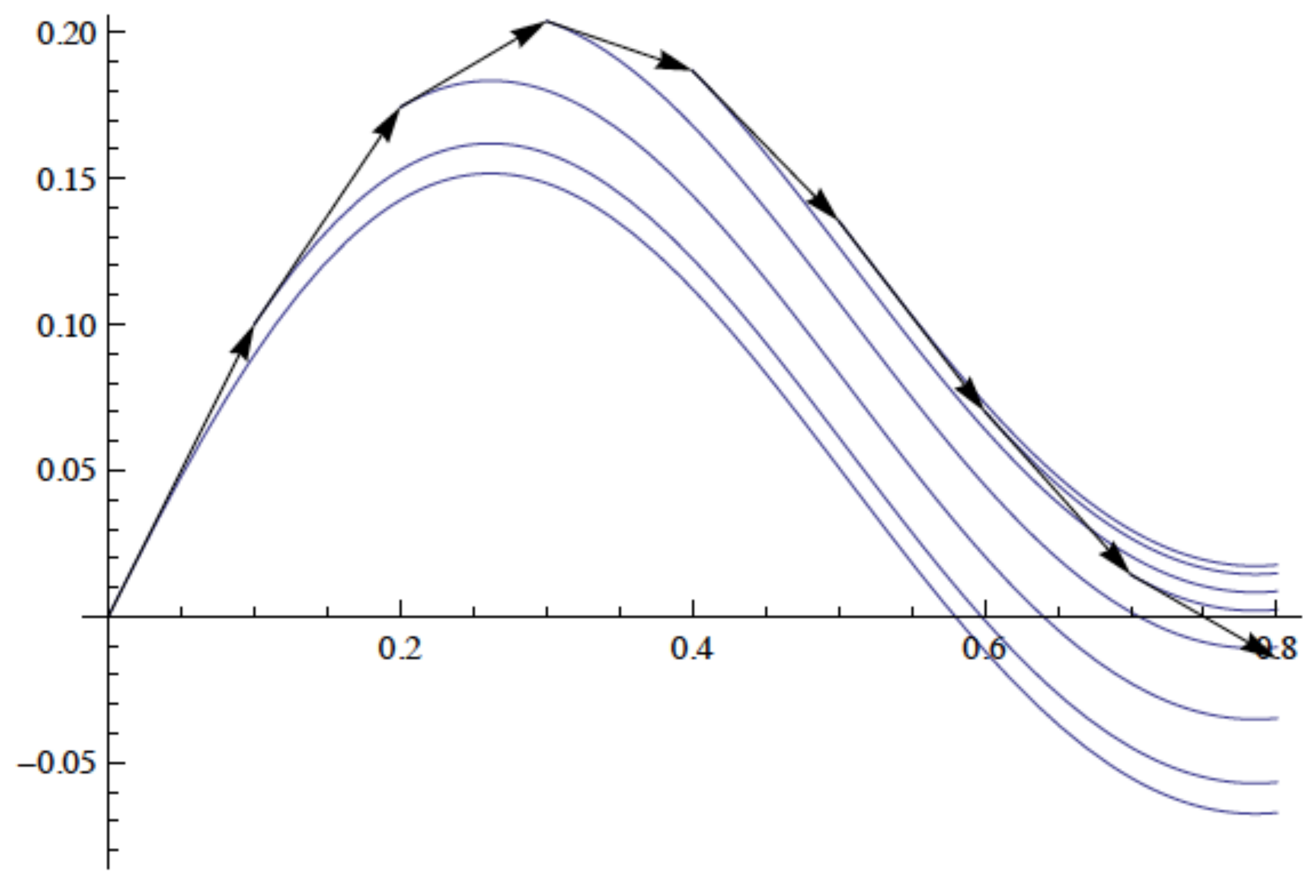


- Exercise: Apply the mean value theorem for the following function $g(t, x) = t\,x + t^2x^2$

$$t x_2 + t^2 x_2^2 - t x_1 - t^2 x_1^2 = (t + 2t^2\xi)(x_2 - x_1)$$

Local and global error

- Even though the **local error** at each step may be quite small, the **total (global) error** may accumulate and become much bigger.



Local and Global Errors

- Basic idea in Euler's method: $\boldsymbol{x_{k+1} = x_k + hf(t_k, x_k)}$ *at* $x(t_{k+1})$
- Approximation: $\boldsymbol{x(t_{k+1}) \approx x_{k+1} = x_k + hf(t_k, x_k)}$
- Simple Taylor Approximation

$$x(t_{k+1}) = x(t_k) + hx'(t_k) + \frac{h^2}{2}x''(\xi_k) = x(t_k) + hf\big(t_k, x(t_k)\big) + \frac{h^2}{2}x''(\xi_k)$$

$\xi_k \in [t_k, t_{k+1}]$

- Global error accumulated: $\epsilon_{k+1} = x(t_{k+1}) - x_{k+1}$

$$x(t_{k+1}) - x_{k+1} = \underbrace{x(t_k) - x_k}_{\epsilon_k} + h\big(f\big(t_k, x(t_k)\big) - f(t_k, x_k)\big) + \underbrace{\frac{h^2}{2}x''(\xi_k)}_{\text{local error}}$$

Local and Global Errors (cont'd)

$$x(t_{k+1}) - x_{k+1} = x(t_k) - x_k + h\big(f\big(t_k, x(t_k)\big) - f(t_k, x_k)\big) + \frac{h^2}{2}x''(\xi_k)$$

- Mean Value Theorem

$$f\big(t_k, x(t_k)\big) - f(t_k, x_k) = f_x(t_k, \theta_k)\big(x(t_k) - x_k\big) = f_x(t_k, \theta_k)\epsilon_k$$

θ_k is a number in the interval $(x_k, x(t_k))$

$$\epsilon_{k+1} = \big(1 + h f_x(t_k, \theta_k)\big)\epsilon_k + \frac{h^2}{2}x''(\xi_k)$$

Local and Global Errors (cont'd)

- If the two first derivatives of f exist, the error in using Euler's method for solving $x' = f(t, x)$ develops according to the relation

$$\epsilon_{k+1} = \big(1 + h f_x(t_k, \theta_k)\big)\epsilon_k + \frac{h^2}{2} x''(\xi_k).$$

- where ξ_k is a number in the interval (t_k, t_{k+1}) and θ_k is a number in the interval x_k, $x(t_k)$.
- The global error at step k + 1 has two sources:
  - The advancement of the **global error** at step k to the next step

$$\big(1 + h f_x(t_k, \theta_k)\big)\epsilon_k$$

  - The **local truncation error** committed by only including two terms in the Taylor polynomial

$$h^2 x''(\xi_k)/2$$

Taylor Methods

Differentiating the differential equations

- **How to determine higher order derivatives of the solution of a differential equation at a point**
  - Example: $x'(t) = t + x^2(t)$, $x(a) = x_0$.
    - At $x = a$: $x(a) = x_0$, $x'(a) = a + x_0^2$.
    - $x''(t) = 1 + 2x(t)x'(t) = 1 + 2x(t)(t + x^2(t))$
    - $x''(a) = 1 + 2x(a)x'(a) = 1 + 2x_0(a + x_0^2)$
    - Higher order derivatives can be determined similarly

Differentiating the differential equations

- Let $x'(t) = f(t, x)$ be a differential equation with initial condition $x(a) = x_0$, and suppose that the derivatives of $f(t,x)$ of order p-1 exist at the point (a, x_0).
- Then the p^{th} derivative of the solution x(t) at x = a can be expressed in terms of a and x_0: $x^{(p)}(a) = F_p(a, x_0)$, where F_p is a function defined by f and its derivatives of order less than p

Exercises

- *Compute x''(a) and x'''(a) of the following differential equations at the given initial value.*

a) $x' = x, \quad x(0) = 1.$

b) $x' = t, \quad x(0) = 1.$

c) $x' = tx - \sin x, \quad x(1) = 0.$

d) $x' = t/x, \quad x(1) = 1.$

Introduction

- Main idea: to approximate the solution by a Taylor polynomial of a suitable degree.
- Euler's method is the simplest Taylor method
  - $x(t + h) \approx x(t) + hx'(t)$
- Quadratic Taylor method approximation
  - $x(t + h) \approx x(t) + h\,x'(t) + (h^2/2)x''(t)$

Quadratic Taylor Method

- The numerical solution advances from a point (t_k,x_k) to a new point (t_{k+1},x_{k+1}) with $t_{k+1} = t_k + h$

$$x_{k+1} = x_k + hx'_k + \frac{h^2}{2}x''_k$$

- Example

$$x' = f(t,x) = F_1(t,x) = t - \frac{1}{1+x}, \quad x(0) = 1$$

  - Apply the quadratic Taylor method on [0,1] with h=0.5

Quadratic Taylor Method (cont'd)

$$x' = f(t,x) = F_1(t,x) = t - \frac{1}{1+x}, \quad x(0) = 1$$

$$x''(t) = F_2(t,x) = 1 + \frac{x'(t)}{(1+x(t))^2}.$$

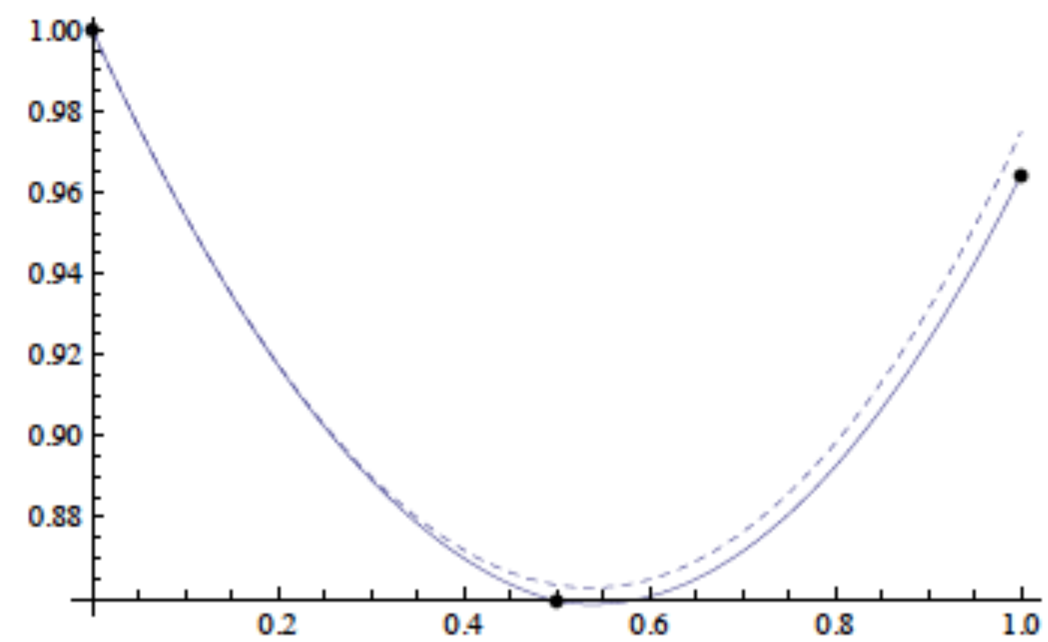
$$x(h) \approx x_1 = x(0) + hx'(0) + \frac{h^2}{2}x''(0)$$

$$x(0) = x_0 = 1,$$
$$x'(0) = x'_0 = 0 - 1/2 = -1/2,$$
$$x''(0) = x''_0 = 1 - 1/8 = 7/8,$$

$$x(h) \approx x_1 = x_0 + hx'_0 + \frac{h^2}{2}x''_0 = 1 - \frac{h}{2} + \frac{7h^2}{16} = 0.859375$$

$$x'(h) \approx x'_1 = F_1(t_1, x_1) = t_1 - 1/(1+x_1) = -0.037815126,$$
$$x''(h) \approx x''_1 = F_2(t_1, x_1) = 1 + x'_1/(1+x_1)^2 = 0.98906216,$$

$$x(1) = x(2h) \approx x_2 = x_1 + hx'_1 + \frac{h^2}{2}x''_1 = 0.96410021$$



Quadratic Taylor Method (cont'd)

- *The quadratic Taylor method advances the solution from a point (t_k, x_k) to a point (t_{k+1}, x_{k+1}) by evaluating the approximate Taylor polynomial at $x = t_{k+1}$*

$$x(t) \approx x_k + (t - t_k)x'_k + \frac{(t - t_k)^2}{2} x''_k$$

- *The new value x_{k+1} is given by*

$$x_{k+1} = x_k + hx'_k + \frac{h^2}{2} x''_k$$

Taylor method of higher degree

- Taylor method of degree p

$$x_{k+1} = x_k + h x'_k + \frac{h^2}{2} x''_k + \cdots + \frac{h^{p-1}}{(p-1)!} x_k^{(p-1)} + \frac{h^p}{p!} x_k^{(p)}$$

Exercises

- Compute numerical solutions to x(1) for the equations below using two steps with Euler's method and the quartic Taylor method. For comparison the correct solution to 14 decimal digits is given in each case.

a) $x' = t^5 + 4, \qquad x(0) = 1,$
$x(1) = 31/6 \approx 5.1666666666667.$

b) $x' = x + t, \quad x(0) = 1,$
$x(1) \approx 3.4365636569181.$

c) $x' = x + t^3 - 3(t^2 + 1) - \sin t + \cos t, \quad x(0) = 7$
$x(1) \approx 13.714598298644.$

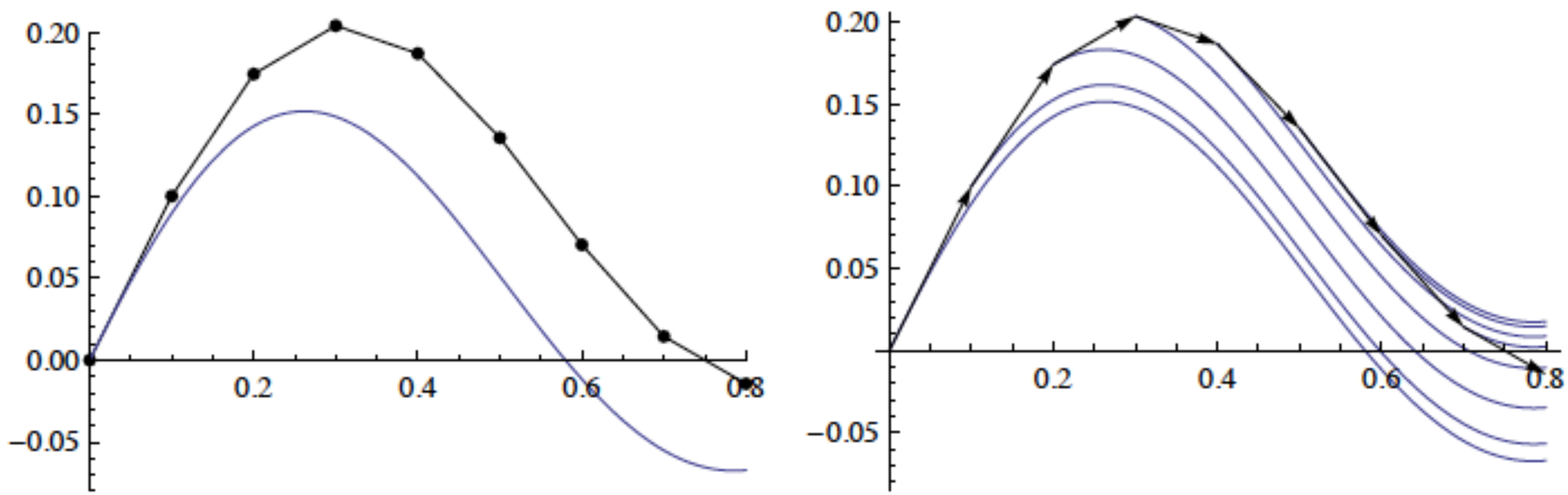
Midpoint Euler and other Runge-Kutta methods

Introduction

- Taylor methods
  - **Advantage**: can attain any approximation order.
  - **Disadvantage:** require **symbolic differentiation** of the differential equation (except for Euler's method).
- Need to develop some methods of higher order than Euler's method that **do not require differentiation of the differential equation**.
  - They advance from (t_k, x_k) to (t_{k+1}, x_{k+1}) by evaluating $f(t,x)$ at intermediate points in the interval $[t_k, t_{k+1}]$.

Euler's midpoint

- Simple improvement of Euler's method.
- The <u>tangent is a good approximation</u> to a solution curve <u>at the initial condition</u>, <u>**But**</u>
- The <u>quality of the approximation</u> deteriorates as we move to the right.



Improvement: estimate the slope of each line segment better.

Euler's midpoint (cont'd)

- Euler's midpoint: two-step procedure which aims to **estimate the slope at the midpoint between the two solution points**.
- In proceeding from (t_k, x_k) to (t_{k+1}, x_{k+1}), **use the tangent to the solution curve at the midpoint $t_k + h/2$**
  - Compute an **approximation $x_{k+1/2}$** to the solution at **$t_k + h/2$** using the traditional Euler's method.
  - Determine the **slope of the solution curve** that passes through the point and **use this as the slope for a straight line** to be followed from t_k to t_{k+1} to determine the new approximation x_{k+1}.

Euler's midpoint (cont'd)

The solution is advanced from (t_k, x_k) *to* $(t_k + h, x_{k+1})$ *in two steps:*

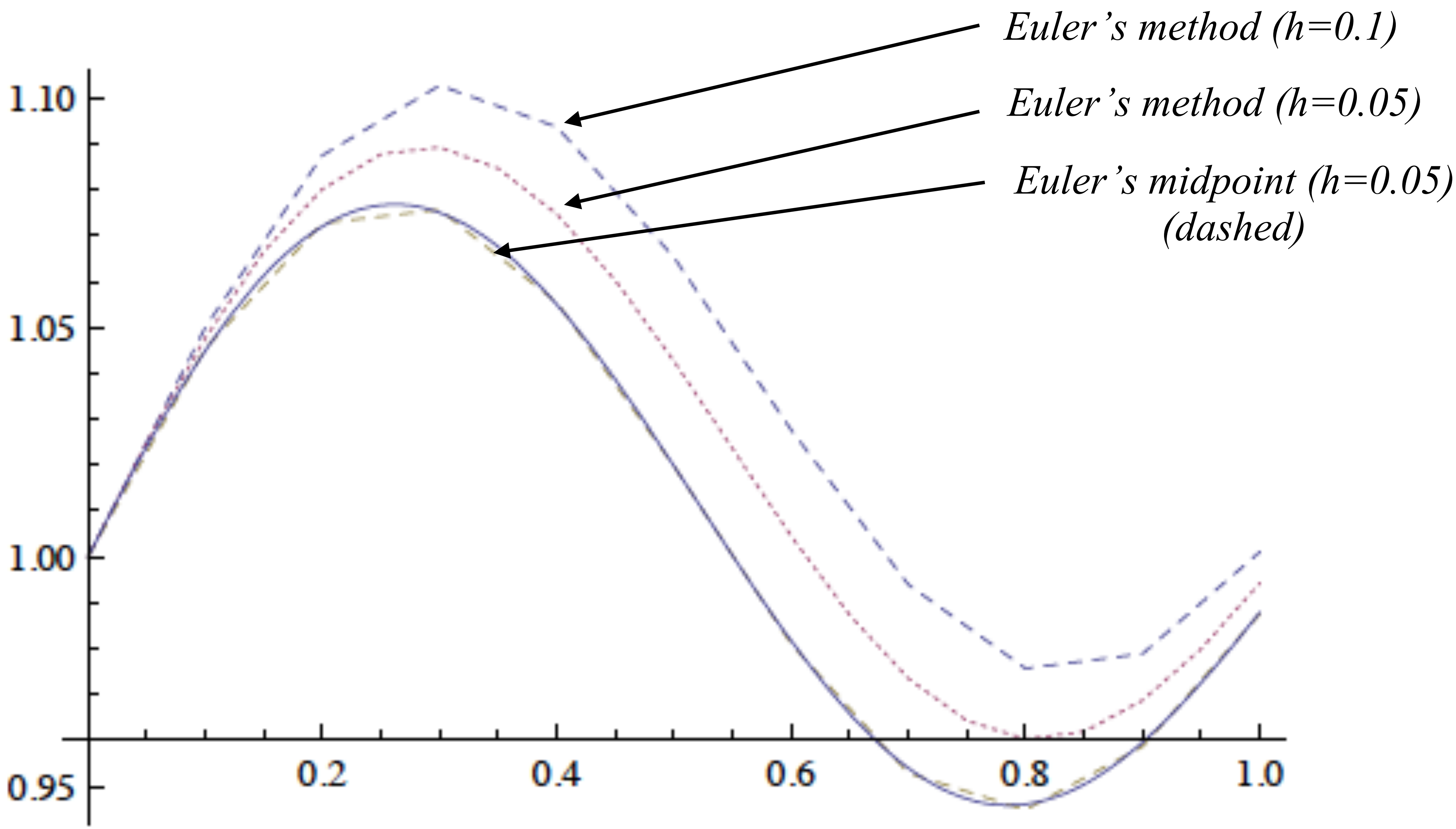
First an approximation to the solution is computed at the midpoint $t_k + h/2$ *by using Euler's method with step length* $h/2$,

$$x_{k+1/2} = x_k + (h/2)\, f(t_k, x_k)$$

Then the solution is advanced to t_{k+1} *by following the straight line from* (t_k, x_k) *with slope given by* $f(t_k + h/2, x_{k+1/2})$

$$x_{k+1} = x_k + h\, f(t_k + h/2, x_{k+1/2})$$

Euler's midpoint (cont'd)



Exercise

Consider the first order differential equation

$$x' = x, \; x(0)=1.$$

a) Estimate x(1) by using <u>one step</u> with Euler's method.

b) Estimate x(1) by using <u>one step</u> with the quadratic Taylor method.

c) Estimate x(1) by using <u>one step</u> with Euler's midpoint method.

$$x_{k+1/2} = x_k + (h/2)\, f(t_k, x_k)$$

$$x_{k+1} = x_k + h\, f(t_k + h/2,\, x_{k+1/2})$$

Runge-Kutta methods

- Runge-Kutta methods are generalizations of the midpoint Euler method.
- The methods use several evaluations of f between each step which leads to higher accuracy.
- Generalized form

$$
\begin{aligned}
&x_{k+1} = x_k + h * \phi(t_k, x_k, h) \\
&\phi = a_1 * k_1 + a_2 * k_2 + ... + a_n * k_n \\
&k_1 = f(t_k, x_k) \\
&k_2 = f(t_k + \lambda_1 * h, x_k + q_{11} * k_1 * h) \\
&k_3 = f(t_k + \lambda_2 * h, x_k + q_{21} * k_1 * h + q_{22} * k_2 * h) \\
&. \\
&. \\
&k_{n+1} = f(t_k + \lambda_n * h, x_k + q_{n1} * k_1 * h + q_{n2} * k_2 * h + ... + q_{nn} * k_n * h)
\end{aligned}
$$

$\boxed{\textbf{RK-1} \Leftrightarrow \textbf{Euler}}$

Second Order Range-Kutta Method

- Second order Range-Kutta

$$x_{k+1} = x_k + h * (a_1 * k_1 + a_2 * k_2)$$
$$k_1 = f(t_k, x_k)$$
$$\boxed{k_2 = f(t_k + \lambda_1 * h, x_k + q_{11} * k_1 * h)}$$

1

- Taylor method (second order)

$$x_{k+1} = x_k + h * f(t_k, x_k) + \frac{h^2}{2!} * f'(t_k, x_k)$$

$$f'(t_k, x_k) = f'_t + f'_x * x'_t$$

$$f'(t_k, x_k) = f'_t + f'_x * f$$

$$\boxed{x_{k+1} = x_k + h * f(t_k, x_k) + \frac{h^2}{2!} * (f'_t(t_k, x_k) + f'_x(t_k, x_k) * f(t_k, x_k))}$$

2

Second Order Range-Kutta Method (cont'd)

- Development using Taylor series

$$f(t+r, x+s) = f(t,x) + r * f_t'(t,x) + s * f_x'(t,x) + \ldots$$

- Applying on k_2

$$k_2 = f(t_k + \lambda_1 * h, x_k + q_{11} * k_1 * h)$$

$$k_2 = f(t_k, x_k) + \lambda_1 * h * f_t'(t_k, x_k) + h * q_{11} * k_1 * f_x'(t_k, x_k) + O(h^2)$$

$$k_2 = f(t_k, x_k) + \lambda_1 * h * f_t'(t_k, x_k) + h * q_{11} * f(t_k, x_k) * f_x'(t_k, x_k) + O(h^2)$$

$$\text{Note: remove } (t_x, x_k) \text{ in the rest for abbreviation}$$

$$x_{k+1} = x_k + h * (a_1 * k_1 + a_2 * k_2)$$

$$x_{k+1} = x_k + h * (a_1 * f + a_2 * (f + \lambda_1 * h * f_t' + h * q_{11} * f * f_x' + O(h^2)))$$

$$\boxed{x_{k+1} = x_k + (a_1 + a_2) * h * f + h^2 * (a_2 * \lambda_1 * f_t' + a_2 * q_{11} * f * f_x') + O(h^3)}$$

3

Second Order Range-Kutta Method (cont'd)

$$x_{k+1} = x_k + h * f + \frac{h^2}{2!} * (f_t' + f_x' * f)$$ 2

$$x_{k+1} = x_k + (a_1 + a_2) * h * f + h^2 * (a_2 * \lambda_1 * f_t' + a_2 * q_{11} * f * f_x') + O(h^3)$$ 3

$$a_1 + a_2 = 1$$
$$2 * a_2 * \lambda_1 = 1$$
$$2 * a_2 * q_{11} = 1$$

$$\Rightarrow$$

$$a_1 = 1 - a_2$$
$$\lambda_1 = q_{11} = \frac{1}{2 * a_2}$$

$$Heun's\ method: a_2 = \frac{1}{2} \Rightarrow a_1 = \frac{1}{2},\ \lambda_1 = q_{11} = 1$$

$$Euler\ Midpoint\ method: a_2 = 1 \Rightarrow a_1 = 0,\ \lambda_1 = q_{11} = \frac{1}{2}$$

$$Ralston's\ method: a_2 = \frac{2}{3} \Rightarrow a_1 = \frac{1}{3},\ \lambda_1 = q_{11} = \frac{3}{4}$$

Second Order Range-Kutta Method (cont'd)

$$x_{k+1} = x_k + h * (a_1 * k_1 + a_2 * k_2)$$
$$k_1 = f(t_k, x_k)$$
$$k_2 = f(t_k + \lambda_1 * h, x_k + q_{11} * k_1 * h)$$

$$a_1 = 1 - a_2$$
$$\lambda_1 = q_{11} = \frac{1}{2*a_2}$$

$Consider\ a_2 = \lambda$

$$\boxed{x_{k+1} = x_k + h * ((1 - \lambda) * f(t_k, x_k) + \lambda * f(t_k + \frac{h}{2 * \lambda}, x_k + \frac{h}{2 * \lambda} * f(t_k, x_k))}$$

Fourth Order Range-Kutta Method

- Suppose the differential equation x'= f (t ,x) with initial condition x(a) = x_0 is given.
- The numerical method given by the formulas is 4th order accurate provided the derivatives of f up to order four are continuous and bounded for t ∈∈ **[a,b]** and x 2 **R** .

$$k_0 = f(t_k, x_k)$$

$$k_1 = f(t_k + \frac{h}{2}, x_k + \frac{h}{2} * k_0)$$

$$k_2 = f(t_k + \frac{h}{2}, x_k + \frac{h}{2} * k_1)$$

$$k_3 = f(t_k + h, x_k + h * k_2)$$

$$x_{k+1} = x_k + \frac{h}{6}(k_0 + 2k_1 + 2k_2 + k_3)$$

Exercise

- Consider the first order differential equation: x'= x, x(0)= 1.
- Estimate x(1) by using one step with RK 4th order method.
- Estimate x(1) by using two steps with the RK 4th order method

$$k_0 = f(t_k, x_k)$$

$$k_1 = f(t_k + \frac{h}{2}, x_k + \frac{h}{2} * k_0)$$

$$k_2 = f(t_k + \frac{h}{2}, x_k + \frac{h}{2} * k_1)$$

$$k_3 = f(t_k + h, x_k + h * k_2)$$

$$x_{k+1} = x_k + \frac{h}{6}(k_0 + 2k_1 + 2k_2 + k_3)$$

Lab Exercise

- Consider the first order differential equation

$$x' = f(t, x) = t^2 + x^3 - x, \quad x(0) = 1.$$

- Write a computer program that implements one of the following methods and use it to estimate the value of x(1) with 10, 100, 1000 and 10000 steps?
  - Euler's method.
  - Quadratic Taylor method.
  - Euler's midpoint method.
  - Runge Kutta fourth order method.