Numerical Differentiation and Integration

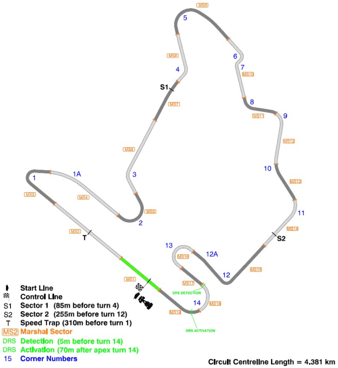
M.Sc. I.M. Manuel F. Mejía De Alba

Maestría en Modelado y Simulación
Universidad Central y Universidad Jorge Tadeo Lozano

Marzo de 2014

Contenido

Introduction problems



The Length of all circuit can be determine by the next expression

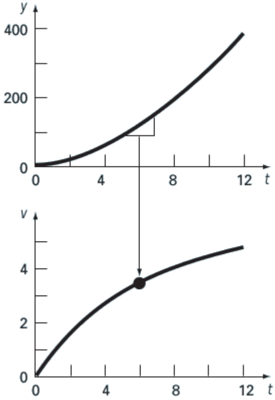
$$\int_{\Omega} \sqrt{1 - \left(\frac{dy}{dx}\right)^2} dx$$

The numerical solution of this problem has sense when the function y is in this forms:

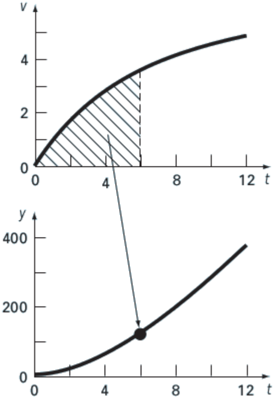
1. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
2. A tabulated function where values of x and f(x) are given at a number of discrete points, as is often the case with experimental or field data.

Mathematical background

Differentiation v. Integration



Differentiation



Integration

Mathematical background

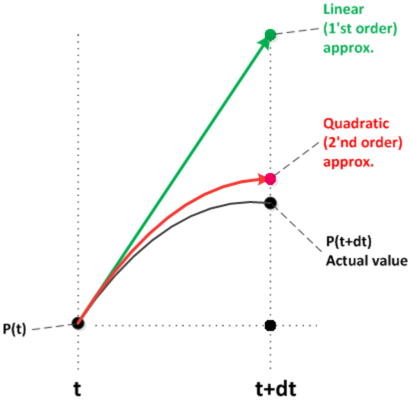
Taylor Serie

$$f(x_{i+1}) = f(x_i) + f'(x_i) * h + \frac{f''(x_i) * h^2}{!2} + \cdots + \frac{f^{(n)}(x_i) * h^n}{!n} + O(h^{n+1})$$

Provides a means to predict a function value at one point in terms of the function value and its derivatives at another point. It is impossible, or practically impossible, the using the exact formulation because is a infinite series. To apply it we have to truncate the series and work with the resulting expression.

It is used to

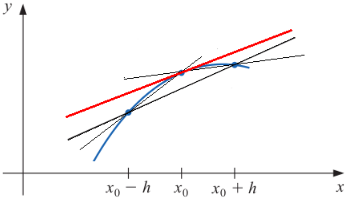
- Estimate numerical errors in another numerical approximations
- To evaluate derivatives (Finite Diference Method)



Mathematical background

Finite differences

$$y' = \frac{dy}{dx} \approx \frac{y_{i+1} - y_i}{dx} \approx \frac{y_i - y_{i-1}}{dx} \approx \frac{y_{i+1} - y_{i-1}}{2dx}$$



In a matrix form, if we have a vector of $y = y_1, \ldots, y_n$ evenly spaced, we can obtain the vector of y'.

$$y' = D' * y$$

$$D' = \frac{1}{dx}\begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 \end{bmatrix} \approx \frac{1}{dx}\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix} \approx \frac{1}{2dx}\begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

By the same way we can generate another D' matrix and moreover $D'', D''' \ldots$

Homework P.1

Differentiation

1. For the next functions plot the error as a function of the number of terms used to make the approximation n. Which scheme of finite diference is better?

   a. $f(x) = e^{2x}$ **b.** $f(x) = x \ln x$
   c. $f(x) = x \cos x - x^2 \sin x$ **d.** $f(x) = 2(\ln x)^2 + 3 \sin x$

   a. $f(x) = e^{2x} - \cos 2x$ **b.** $f(x) = \ln(x + 2) - (x + 1)^2$
   c. $f(x) = x \sin x + x^2 \cos x$ **d.** $f(x) = (\cos 3x)^2 - e^{2x}$

2. Using the code of Newton methods (for one and several variable) already programed by you in the first Homework, add the function to evaluate the derivative using the best scheme of finite differences.

Mathematical background

Numerical Integration

We have the aim of resolve:

$$\int_a^b f(x)dx \approx \int_a^b f^n(x)dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

Newton Cotes closed formulas

Segments (*n*)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b-a)\,\dfrac{f(x_0)+f(x_1)}{2}$	$-(1/12)h^3 f''(\xi)$
2	3	Simpson's 1/3 rule	$(b-a)\,\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-(1/90)h^5 f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b-a)\,\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-(3/80)h^5 f^{(4)}(\xi)$
4	5	Boole's rule	$(b-a)\,\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-(8/945)h^7 f^{(6)}(\xi)$
5	6		$(b-a)\,\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-(275/12{,}096)h^7 f^{(6)}(\xi)$

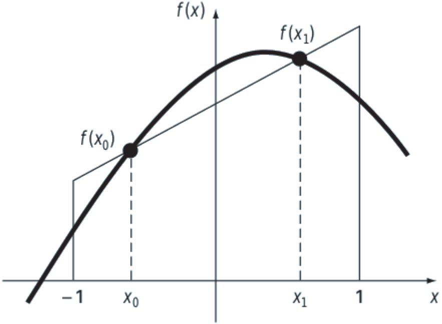
The step size is given by $h = (b-a)/n$.

UNIVERSIDAD CENTRAL

Mathematical background

Numerical Integration

Gauss quadrature



Mathematical background

Numerical Integration

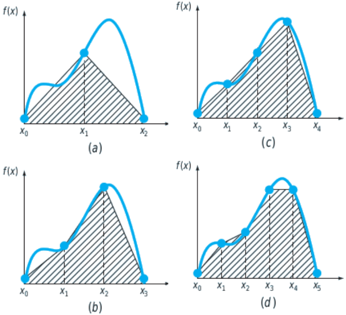
Gauss quadrature

Points	Weighting Factors	Function Arguments	Truncation Error
2	$c_0 = 1.0000000$	$x_0 = -0.577350269$	$\cong f^{(4)}(\xi)$
	$c_1 = 1.0000000$	$x_1 = 0.577350269$	
3	$c_0 = 0.5555556$	$x_0 = -0.774596669$	$\cong f^{(6)}(\xi)$
	$c_1 = 0.8888889$	$x_1 = 0.0$	
	$c_2 = 0.5555556$	$x_2 = 0.774596669$	
4	$c_0 = 0.3478548$	$x_0 = -0.861136312$	$\cong f^{(8)}(\xi)$
	$c_1 = 0.6521452$	$x_1 = -0.339981044$	
	$c_2 = 0.6521452$	$x_2 = 0.339981044$	
	$c_3 = 0.3478548$	$x_3 = 0.861136312$	
5	$c_0 = 0.2369269$	$x_0 = -0.906179846$	$\cong f^{(10)}(\xi)$
	$c_1 = 0.4786287$	$x_1 = -0.538469310$	
	$c_2 = 0.5688889$	$x_2 = 0.0$	
	$c_3 = 0.4786287$	$x_3 = 0.538469310$	
	$c_4 = 0.2369269$	$x_4 = 0.906179846$	
6	$c_0 = 0.1713245$	$x_0 = -0.932469514$	$\cong f^{(12)}(\xi)$
	$c_1 = 0.3607616$	$x_1 = -0.661209386$	
	$c_2 = 0.4679139$	$x_2 = -0.238619186$	
	$c_3 = 0.4679139$	$x_3 = 0.238619186$	
	$c_4 = 0.3607616$	$x_4 = 0.661209386$	
	$c_5 = 0.1713245$	$x_5 = 0.932469514$	

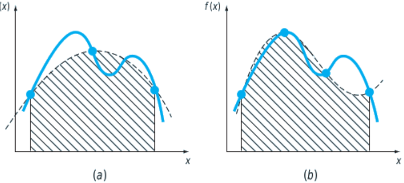
Mathematical background

Numerical Integration

How to improve the results ?



h-refinement



p-refinement

Homework P.1

Differentiation

1. For the next functions plot the error as a function of the number of terms used to make the approximation n. Which formula quadrature is better?

a.	$f(x) = e^{2x}$	**b.**	$f(x) = x \ln x$
c.	$f(x) = x \cos x - x^2 \sin x$	**d.**	$f(x) = 2(\ln x)^2 + 3 \sin x$
a.	$f(x) = e^{2x} - \cos 2x$	**b.**	$f(x) = \ln(x+2) - (x+1)^2$
c.	$f(x) = x \sin x + x^2 \cos x$	**d.**	$f(x) = (\cos 3x)^2 - e^{2x}$