Numerical methods – lecture 9

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Numerical calculation of the derivative

$x_0, \ldots, x_n$ – given points,
$f_0, \ldots, f_n$ – given function values, $f_k = f(x_k)$

We want to calculate the approximation of $f'(x)$ from this data.

Let P be the interpolation polynomial for given data.

$$f'(x) \approx P'(x)$$

Example 1.

$n = 1$,
Data: $x_0, x_1,\ f_0, f_1$

$P(x) = \frac{f_1 - f_0}{x_1 - x_0}(x - x_0) + f_0$

$f'(x) \approx P'(x) = \frac{f_1 - f_0}{x_1 - x_0}$

Example 2.

$n = 2$, data: $x_0, x_1, x_2,\ f_0, f_1, f_2$

$$P(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$P'(x) = f_0 \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

Equidistant points: $x_1 - x_0 = x_2 - x_1 = h$:

$$P'(x) = f_0 \frac{2x-x_1-x_2}{2h^2} - f_1 \frac{2x-x_0-x_2}{h^2} + f_2 \frac{2x-x_0-x_1}{2h^2}$$

$$P'(x_0) = \frac{1}{2h}(-3f_0 + 4f_1 - f_2)$$

$$P'(x_1) = \frac{1}{2h}(f_2 - f_0)$$

$$P'(x_2) = \frac{1}{2h}(f_0 - 4f_1 + 3f_2)$$

$$P''(x) = \frac{1}{h^2}(f_0 - 2f_1 + f_2)$$

Derivation from the Taylor series

$$\begin{aligned}
I: &\quad f(x+h) = f(x) + f'(x)h + \tfrac{1}{2}f''(x)h^2 + \tfrac{1}{6}f'''(x)h^3 + O(h^4) \\
II: &\quad f(x-h) = f(x) - f'(x)h + \tfrac{1}{2}f''(x)h^2 - \tfrac{1}{6}f'''(x)h^3 + O(h^4) \\
I\text{–}II: &\quad f(x+h) - f(x-h) = 2f'(x)h + \tfrac{1}{3}f'''(x)h^3 + O(h^4) \\
&\quad f'(x) = \tfrac{1}{2h}[f(x+h) - f(x-h)] + O(h^2) \\
I{+}II: &\quad f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + O(h^4) \\
&\quad f''(x) = \tfrac{1}{h^2}[f(x+h) - 2f(x) + f(x-h)] + O(h^2)
\end{aligned}$$

Numerical integration – quadrature formulae

$x_0, \dots, x_n$ – given points, $a \le x_0 < x_1 < \dots < x_n \le b$
$f_0, \dots, f_n$ – given function values, $f_k = f(x_k)$

Let P be the interpolation polynomial for given data.

$$\int_a^b f(x)dx \approx \int_a^b P(x)dx$$

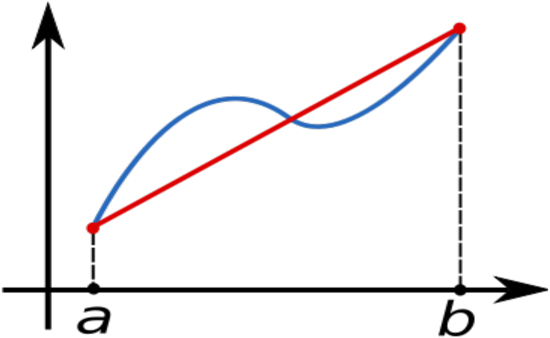
Example 1.

$n = 1,\ a = x_0, b = x_1,\ f(a), f(b)$

$P(x) = \frac{f(b)-f(a)}{b-a}(x-a) + f(a)$

$\int_a^b P(x)dx = \left[\frac{f(b)-f(a)}{b-a}\frac{(x-a)^2}{2} + f(a)x\right]_a^b = \frac{f(a)+f(b)}{2}(b-a)$

Trapezoidal rule



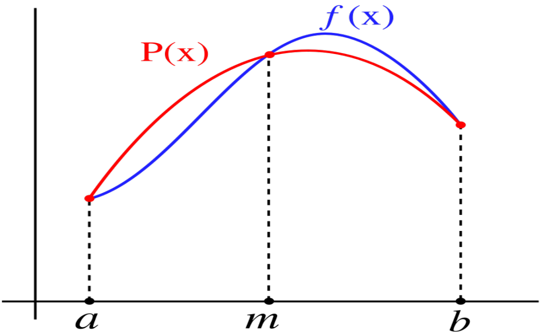
Example 2.

$n = 2$, equidistant points:
$a = x_0, x_1 = a + h = \frac{a+b}{2}, b = x_2 = a + 2h$,
f_0, f_1, f_2 – function values

$$P(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$\begin{aligned} \int_a^b f(x)dx \approx \int_a^b P(x)dx &= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \\ &= \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \end{aligned}$$

Simpson's rule



Composite (chained) trapezoidal rules

Equidistant points:

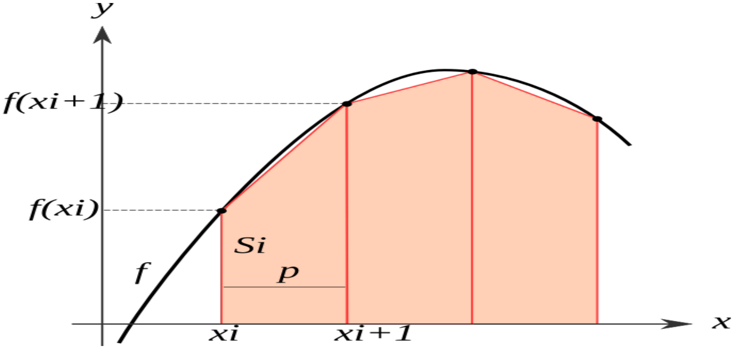
$a = x_0 < x_1 < \cdots < b = x_n,\ x_{i+1}` = x_i + h,\ f_i = f(x_i)$

We use the trapezoidal rule for every interval $[x_i, x_{i+1}]$:

$$\int_a^b f(x)dx \approx$$

$$\approx \frac{f_0 + f_1}{2}h + \frac{f_1 + f_2}{2}h + \frac{f_2 + f_3}{2}h + \cdots + \frac{f_{n-1} + f_n}{2}h =$$

$$= \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n]$$


y
f(xi+1)
f(xi)
Si
p
f
xi
xi+1
x

Composite Simpson's rules

Equidistant points, n – even:

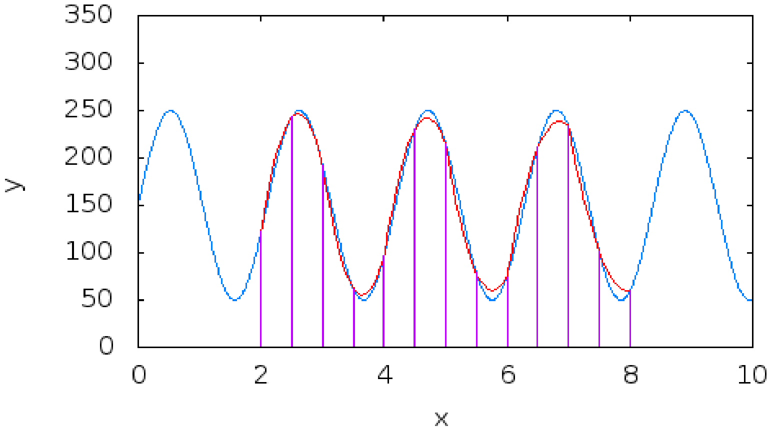
$a = x_0 < x_1 < \cdots < b = x_n$, $x_{i+1}` = x_i + h$, $f_i = f(x_i)$

We use the Simpson's rule for every interval $[x_{2i}, x_{2i+2}]$:

$$\int_a^b f(x)dx \approx$$

$$\approx \frac{h}{3}[f_0 + 4f_1 + f_2] + \frac{h}{3}[f_2 + 4f_3 + f_4] + \cdots + + \frac{h}{3}[f_{n-2} + 4f_{n-1} + f_n]$$

$$= \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 2f_{n-2} + 4f_{n-1} + f_n]$$



350
300
250
200
150
100
50
0
y
0
2
4
6
8
10
x

Monte Carlo integration

Method I

$X_1, \ldots, X_n$ – random numbers distributed uniformly on $[a, b]$

$$\int_a^b f(x)dx \approx \frac{b-a}{n}\sum_{i=1}^{n} f(X_i)$$

Monte Carlo integration

Method II

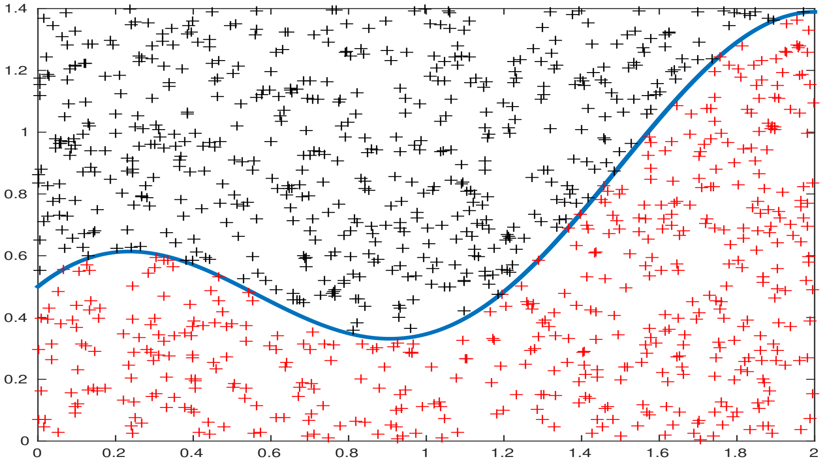
Let f be non-negative on $[a, b]$, $f(x) \leq M$ for every $x \in [a, b]$.

$[X_1, Y_1]$,…,$[X_n . Y_n]$ – observations of the random vector $[X, Y]$ distributed uniformly on $[a, b] \times [0, M]$

$$P(Y \leq f(X)) = \frac{\int_a^b f(x)dx}{M(b-a)} \approx \frac{1}{n} \sum_{i=1}^{n} I_{Y_i \leq f(X_i)}$$

where I is the indicator function.

$$\int_a^b f(x)dx \approx \frac{M(b-a)}{n} \sum_{i=1}^{n} I_{Y_i \leq f(X_i)}$$

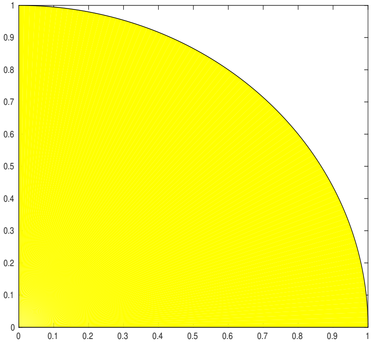


1.4
1.2
1
0.8
0.6
0.4
0.2
0
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8 2

Application:

Approximation of π:
$[X, Y]$ distributed uniformly on $[0,1] \times [0,1]$

$P(X^2 + Y^2 \leq 1) = \frac{\pi}{4}$



$[X_1, Y_1]$,...,$[X_n.Y_n]$: observations of $[X, Y]$

$$\pi \approx \frac{4}{n} \sum_{i=1}^{n} I_{Y_i^2 + X_i^2 \leq 1}$$