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Quadrature methods (I) Solutions

Exercice 1 (Lagrange interpolation).

Let f be a smooth function over $[a, b]$. Let $x_0, \ldots, x_n \in [a, b]$ (all distinct). The Newton polynomial basis is defined as :

$$w_{n+1} = \prod_{i=0}^{n}(X - x_i)$$

with the convention that w_0 is the constant polynomial $w_0 = 1$. The Lagrange interpolation of f based on the nodes $x_0, \ldots, x_n$ is defined as :

$$L_n f = \sum_{i=0}^{n} f(x_i) l_i \quad \text{where} \quad l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

1. Assume that f is differentiable $(n + 1)$ times on $[a, b]$. Show that for all $x \in [a, b]$ there exists $c_x \in [a, b]$ such that the interpolation error $e_n(x)$ can be written :
$$e_n(x) = f(x) - L_n f(x) = \frac{1}{(n + 1!)} w_{n+1}(x) f^{(n+1)}(c_x)$$
Hint : find the appropriate function on which to apply generalized Rolle's theorem
To minimize the error, we can chose the nodes that minimize the values of $w_n(x)$.
2. Consider the equidistant nodes sequence $x_i = a + i\frac{b-a}{n}$. Show that :
$$\|w_n\|_\infty \leq (n + 1)! \left(\frac{b - a}{n}\right)^n$$
3. Refine that upper-bound to obtain using Sterling's formula.
The proof of the previous result highlights the fact that the amplitude of w_n is larger near the borders of the interval or when the nodes are too far from each other. To counteract this effect, we can pick nodes that get denser around the borders. Such nodes can be given by the roots of the Tchebychev polynomials defined by :
$$T_n(x) = \cos(n \arccos(x))$$
4. Show that T_n verify the recurrence :
$$T_0(x) = 1 \qquad T_1(x) = x \qquad T_{n+1}(x) + T_{n-1}(x) = 2xT_n(x), \quad n \geq 1$$
and deduce the degree, the roots and the coefficient of the leading term of T_n.
5. Let $u_0, \ldots, u_{n+1}$ denote the roots of T_n. Let $\phi : [-1, 1] \to [a, b]$ be the affine transformation $u \mapsto \frac{b-a}{2}u + \frac{a+b}{2}$. Define the Tchebychev interpolation nodes $x_k = \phi(u_k)$. Show that :
$$\|w_n^{Tch}\| \leq 2\left(\frac{b - a}{4}\right)^n$$

Exercice 2 (Cavalieri-Simpson).
Let f be a smooth (C^∞) function over $[a, b]$. We consider the problem of evaluating the integral $I(f) = \int_a^b f(x)\, \mathrm{d}x$. We approximate $I(f)$ using a simple quadrature method of Newton-Cotes of order l with the nodes : $x_i = a + i\frac{b-a}{l}$, $i = 0, \ldots, l$, and weights $\lambda_0, \ldots, \lambda_l$, such that :

$$\hat{I}(f) = (b - a)\sum_{i=0}^{l} \lambda_i f(x_i)\,.$$

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1. Show that the weights λ_i are independent of (a, b). Without loss of generality, we can assume that $(a, b) = (-1, 1)$.
2. Find λ_i for $l = 2$.
3. Show that this quadrature method is of order 3.

Exercice 3 (Legendre-Gauss quadrature)**.**
Let $I(f) = \int_{-1}^{1} f$, where f is a smooth function over $[-1, 1]$. Let $u_0, u_1 \in [-1, 1]$. We are interested in a rule of the form :

$$\lambda_0 f(u_0) + \lambda_1 f(u_1).$$

In this exercise, the interpolation nodes are not fixed. Find $(u_0, u_1, \lambda_0, \lambda_1)$ so as to maximize the order of the method.

Exercice 4 (Gauss-Newton)**.**

Consider the problem of approximating $I_{a,b}(f) = \int_a^b f(x)\,\mathrm{d}x$, where f is in $\mathcal{C}^\infty$ via

$$\hat{I}_{a,b}(f) = (b - a)(\lambda_0 f(a) + \lambda_1 f(b) + \lambda_2 f'(a)),$$

with $(\lambda_0, \lambda_1, \lambda_2) \in \mathbb{R}^3$.

1. For $a = 0$, $b = 1$, find $(\lambda_0, \lambda_1, \lambda_2)$ such that the order of the method is exact for polynomials of degree ≤ 2.
2. Deduce an expression of $(\lambda_0, \lambda_1, \lambda_2)$ as function of a and b such that the method is of order 2 for any interval $[a, b]$.

Solutions

Ex 1

1. Let $x \in [a,b]$. Consider adding a new node x_{n+1} set to x which defines the interpolation $L_{n+1}f$. Therefore one can write :
$$e_n(x) = f(x) - L_n f(x) = L_{n+1}f(x) - L_n f(x)$$
Since all the nodes $x_0, \dots, x_n$ are common between $L_n f$ and $L_{n+1}f$, the polynomial $L_{n+1}f - L_n f$ is of degree lower than $n+1$ and has $x_0, \dots, x_n$ as roots. Therefore, there exists $A > 0$ such that : $e(x) = f(x) - L_n f(x) = Aw_{n+1}(x)$. Now define the function :
$$g : t \mapsto f(t) - L_n f(t) - Aw_{n+1}(t)$$
. It holds $g(x_i) = 0$ for all $i \leq n+1$ therefore by Rolle's generalized theorem : there exists $c_x \in [a,b]$ such that :
$$\begin{aligned} g^{(n+1)}(c_x) = 0 &\Rightarrow f^{(n+1)}(c_x) - A(n+1)! = 0 \\ &\Rightarrow A = \frac{f^{(n+1)}(c_x)}{n+1!} \end{aligned}$$
Substituting A in $g(x) = g(x_{n+1}) = 0$ leads to the result.
2. Let $x \in [a,b]$. Denote by $\iota(x)$ the element i such that $x \in [x_i, x_{i+1}[$. Denote the regular interval diameter by $\Delta = \frac{b-a}{n}$. It holds :
$$|x - x_j| \leq |j - i(x) + 1|\Delta$$
We would like to have an inequality independent of x. It is straightforward to do so *after* taking the product. Since $i(x) \in [|0,n|]$: $|w_{n+1}(x)| = \prod_{j=0}^n |x - x_j| \leq \prod_{j=0}^n |j - i(x) + 1|\Delta \leq \prod_{j=0}^n |j+1|\Delta = (n+1)!\Delta^n$.
3. Using Sterling's formula $n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ leads to the upper-bound :
$$O\left(\sqrt{n}\left(\frac{b-a}{e}\right)^n\right)$$
4. Let $\alpha = \arccos(x) \in [0, \pi]$.
$$\begin{aligned} T_{n+1}(x) + T_{n-1}(x) &= \cos((n+1)\alpha) + \cos((n-1)\alpha) \\ &= \cos(n\alpha)\cos(\alpha) - \sin(n\alpha)\sin(\alpha) + \cos(n\alpha)\cos(\alpha) + \sin(n\alpha)\sin(\alpha) \\ &= 2\cos(n\alpha)\cos(\alpha) \\ &= 2x\cos(n\alpha) \\ &= 2xT_n(x) \end{aligned}$$
The recurrence formula shows that $\deg(T_n) = n$, the leading coefficient of T_n is 2^{n-1} and that the roots of T_n are given by :
$$\begin{aligned} T_n(u) = 0 &\Rightarrow \cos(n \arccos(u)) = 0 \\ &\Rightarrow n\arccos(u) = \frac{\pi}{2} + k\pi \text{ for some } k \in [|0, n-1|] \\ &\Rightarrow u = \cos\left(\frac{2k+1}{2n}\pi\right) \text{ for some } k \in [|0, n-1|] \end{aligned}$$
5. Applying ϕ leads to the (n+1) nodes : $x_i = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{2k+1}{2n+2}\pi\right)$. Let $x \in [a,b]$. It holds that : $x - x_i = \frac{b-a}{2}(u - u_i)$ where $u = \phi^{-1}(x)$. Therefore :
$$w_{n+1}(x) = \left(\frac{b-a}{2}\right)^n \prod_{i=0}^n (u - u_i)$$

$$
\begin{aligned}
&= \left(\frac{b-a}{2}\right)^n \frac{1}{2^n} t_n(u) \\
&= 2\left(\frac{b-a}{4}\right)^n t_n(u)
\end{aligned}
$$

Since $|t_n(u)| \leq 1$, it holds :

$$
|w_{n+1}|_\infty = 2\left(\frac{b-a}{4}\right)^n
$$

Ex 2

1. We consider the usual change of variable $\phi : u \in [-1, 1] \mapsto \frac{a+b}{2} + \frac{b-a}{2}u$. The weights λ_i are defined by the Integral of the Lagrange interpolation. Indeed, if the approximation of f by $L_n f$ then :

$$
\frac{1}{b-a}\int_a^b f = \frac{1}{b-a}\int_a^b \sum_{i=0}^n f(x_i) l_i(x) = \frac{1}{b-a}\sum_{i=0}^n \int_a^b l_i(x)
$$

thus λ_i must verify :

$$
\lambda_i = \frac{1}{b-a}\int_a^b l_i(x)
$$

. Using the definition of l_i and the change of variable above leads to the result :

$$
\lambda_i = 2\int_{-1}^1 \prod_{j\neq i} \frac{u-u_i}{u_i-u_j} du
$$

where $u_i = -1 + \frac{2}{n}i$.

2. For $n = 2$ the nodes are given by (-1, 0, 1). The method is exact for polynomials of degree at least 2. Therefore, taking $f = 1$ then $f(x) = x$ then $f(x) = x^2$ leads to :

$$
\begin{aligned}
1 &= \lambda_0 + \lambda_1 + \lambda_2 \\
0 &= -\lambda_0 + \lambda_2 \\
\frac{1}{3} &= \lambda_0 + \lambda_2
\end{aligned}
$$

The solution is given by : $\lambda_0 = \lambda_2 = \frac{1}{6}$ and $\lambda_1 = \frac{2}{3}$. Thus the general rule can be written :

$$
\frac{(b-a)}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)
$$

3. The formula is exact for a cubic $f(x) = x^3$ but not for $f(x) = x^4$. Thus, the method is of order 3.

Ex 3 If $u_0 \neq u_1$, the order of the rule is at least 1 (since one can interpolate straight lines with 2 points). Therefore, taking f constant and f = Id leads to $\lambda_0 + \lambda_1 = 1$ and $\lambda_0 u_0 + \lambda_1 u_1 = 0$. Since the interval $[0, 1]$ is symmetric, it must hold : $u_0 = -u_1$ and $\lambda_0 = \lambda_1$ which leads to $u_0 = \frac{1}{\sqrt{3}}$ and $\lambda_0 = \frac{1}{2}$. Let's see if the rule holds for higher degree polynomials. For f : $x \mapsto x^2$, the exact integral is $\frac{1}{2}\int_{-1}^1 x^2 dx = \frac{1}{3}$ and $\frac{1}{2}\left(\frac{1}{\sqrt{3}}\right)^2 + \frac{1}{2}\left(\frac{1}{\sqrt{3}}\right)^2 = \frac{1}{3}$. For f : $x \mapsto x^3$, the rule trivially holds since $u_0 = -u_1$ and the function is odd. Therefore, by linearity of the integral, the rule holds for any polynomial of degree lower or equal than 3. For f : $x \mapsto x^4$ the integral is $\frac{1}{2}\int_{-1}^1 x^4 dx = \frac{1}{5}$ and the rule gives : $\frac{1}{2}\left(\frac{1}{\sqrt{3}}\right)^4 + \frac{1}{2}\left(\frac{1}{\sqrt{3}}\right)^4 = \frac{1}{9}$. The order of the method is 3.

Remark : Without the symmetry argument, we can retrieve $u_0 = -u_1$ and by taking the polynomials $(X - u_0)(X - u_1)$ and $X(X - u_0)(X - u_1)$.