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Quadrature methods (II)

Exercice 1 (Simple vs composite rules)**.** So far we've seen simple quadrature rule where the integral $\int_a^b f$ is approximated by a weighted sum of the form $(b-a)\sum_{i=0}^n w_i f(x_i)$ where the w_i are obtained by using the Lagrange interpolation of f. Such an approximation is proportional to $(b-a)^n$ and $|f^{(n)}|$ (if f is smooth enough). Using large values of n is in general not a good idea (cf Runge phenomenon). To approximate integrals, it is thus better to use small values of n over multiple and small segments $[a_i, b_i]$: i.e approximate f using a piecewise polynomial interpolation : composite rules.

The simple trapezoidal rule is defined as : $I_{a,b} = (b-a)(\frac{1}{2}f(a) + \frac{1}{2}f(b))$. Let's divide $[a,b]$ into M segments with regular size $h = \frac{b-a}{M}$. Let $a_j = a + jh$, $j \in [|0, M|]$. The composite trapezoidal rule integrates f by applying the simple trapezoidal over each segment of size h. Find the weights w_j such that the composite trapezoidal rule can be written :

$$h\sum_{j=0}^{M} w_j f(a_j)$$

Exercice 2 (Legendre-Gauss quadrature : example)**.**
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 3 (Gaussian quadrature : general case)**.**
Let $\mathcal{X} \subset \mathbb{R}$. Let w be a non-negative weight function (i.e $\int_{\mathcal{X}} \omega = 1$). For any polynomials P, Q defined over $\mathcal{X}$, their scalar product for the weight function w is defined by :

$$\langle P, Q\rangle_\omega = \int_{\mathcal{X}} P(x)Q(x)w(x)\mathrm{d}x.$$

Let f be a continuous function over $\mathcal{X}$. We are interested in finding the optimal weights $(w_i)_i$ and nodes $(x_i)_i$ maximizing the order of the quadrature rule for the integral $I(f) = \int_{\mathcal{X}} \omega f$ given by :

$$\widehat{I_n(f)} = \sum_{i=0}^{n} w_i f(x_i)$$

Part I. Theory

Orthogonal Polynomials. Consider the orthogonal family of polynomials $(P_0, P_1, \dots)$ obtained by applying the Gram-Schmidt process to the basis $1, X, X^2, \dots$ with the inner product $\langle ., . \rangle_\omega$ and the normalization condition $P_n(1) = 1$. First, we prove an important property of any orthogonal family of polynomials : each element P_i has i distinct simple roots in $\mathcal{X}$.

1. Show that P_n changes sign at least once in $\mathcal{X}$.
2. Let $y_1, \dots, y_j$ the only points in $\mathcal{X}$ where P_n changes its sign. Show that $j = n$ and conclude.

Now we move on to show that the maximum order of the method is $2n+1$ and that the nodes are unique and given by the roots of the orthogonal polynomial basis.

Necessary conditions. Assume the rule is of order $2n+1$.

3. Using a particular choice for f, show that the nodes $(x_i)_i$ must be roots of P_{n+1}.
4. Conclude the uniqueness of $(x_i)_i$ and $(w_i)_i$.

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Sufficient conditions.

5. Using Euclidean division, show that the necessary conditions are sufficient for the rule to be of order at least $2n+1$.
6. Using a specific choice of f, show that the order of the rule cannot be larger than $2n+1$.

Examples Let $n = 1$.

— For $\mathcal{X} = [-1, 1]$ and $w(x) = \frac{1}{2}$, $(P_0, P_1, \dots)$ are called the Legendre polynomials.
— For $\mathcal{X} = \mathbb{R}$ and $w(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$. $(P_0, P_1, \dots)$ are called the Hermite polynomials.
— For $\mathcal{X} = [0, +\infty]$ and $w(x) = e^{-x}$, $(P_0, P_1, \dots)$ are called the Laguerre polynomials.

7. Find P_0, P_1 and P_2. Deduce the corresponding Gauss-Legendre quadrature for $n = 1$.

Part II. Implementation In the following questions, you may use library functions referring to polynomials such as `scipy.special.roots_legendre`, `scipy.special.roots_laguerre`, etc ...

8. For $\mathcal{X} = [a, b]$, what change of variable should be applied to the nodes x_i ?
9. Implement a function `def gauss_legendre_simple(f, a, b, nodes, weights)` that approximates the integral of a function f over $[a, b]$ using the Gaussian-Quadrature rule. Test your implementation on some analytically integrable function of your choice.
10. Implement a function `def gauss_legendre(f, n, M, a, b)` that performs the composite rule of Gauss-Legendre over M sub-intervals of [a, b].
11. Write an identical function but with a vectorized implementation `gauss_legendre_vectorized(f, n, M, a, b)` with numpy (does not contain any loop or list comprehensions. Hint : it should not call `gauss_legendre_simple`).
12. Visualize in one plot the integration error of $\int_2^5 \frac{1}{x}$ as a function of both n and M.
13. Write a function `def trapezoidal` that computes the composite trapezoidal rule of Ex 1. Compare the integration error with the Gauss-Legendre method with the same values of M and the number of nodes. What do you conclude ?
14. **Mini-project** Implement different Gauss-quadrature rules (different set of nodes i.e different space $\mathcal{X}$) that approximate the probability $\mathbf{P}(X \leq a)$ for a Gaussian random variable $X \sim \mathcal{N}(0, 1)$ and some $a \in \mathbb{R}$. Evaluate the accuracy of your approximation (as a function of n) using `scipy.stats.norm.cdf`. Which rule is more accurate and why ?

Part III. Richardson acceleration and Romberg's method Consider an approximation $A(h)$ of a quantity of interest A given by :

$$A(h) = A + a_1 h + a_2 h^2 + O(h^k)$$

The goal of Richardson's method is to eliminate the h^i terms using multiple evaluations $A(h_1), A(h_2), \dots$. Let α be a known and fixed positive constant. Setting $h_i = \alpha^i h$ for some $h > 0$, we define :

$$B(h) = \frac{A(\alpha h) - \alpha A(h)}{1 - \alpha} = A + O(h^2)$$

Thus, B eliminates the error term $a_1 h$. This process can be repeated to eliminate the remaining terms.

14. Let $A_{i,0} = A(\alpha^i h)$ and $A_{1,1} = B(h)$. Show that the expression given by $A_{i,j} = \frac{A_{i,j-1} - \alpha^j A_{i-1,j-1}}{1-\alpha^j}$ removes the first j error terms using i nodes.
15. Richardson's acceleration applied to the trapezoidal rule is called Romberg's integration. The error of the trapezoidal rule is given by :

$$\widehat{I_t(h)} = \int f + \sum_{k=1}^{n} a_k h^{2k} + O(h^{2n+2})$$

Implement Richardson's method applied to $I_t(h)$.

16. Plot the integration error as a function of $1/h$ for the trapezoidal rule with and without Richardson's acceleration. Compare with Gaussian quadrature.

Richardson acceleration can also be applied to speed-up optimization algorithms :
https://francisbach.com/richardson-extrapolation/

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Solutions

Ex 1 The linearity of the integral operator leads to :

$$\int_a^b f = \sum_{j=0}^{M-1} \int_{a_j}^{a_{j+1}} f$$

Each small integral $\int_{a_j}^{a_{j+1}} f$ can be approximated using the simple trapezoidal rule :

$$\widehat{I}_{[a_j,a_{j+1}]}(f) = (a_{j+1} - a_j)(f(a_j) + f(a_{j+1})) = h(f(a_j) + f(a_{j+1}))$$

Therefore, the composite rule is given by :

$$\sum_{j=0}^{M-1} \widehat{I}_{[a_j,a_{j+1}]}(f) = \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{M-1} f(a_j) + f(b)\right)$$

Ex 2 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 $X(X - u_0)(X - u_1)$.

Ex 3

1. For $n > 0$, it holds $\langle P_n, 1\rangle = 0$ thus $\int P_n w = 0$. Since w is non-negative, P_n must change its sign at least once.
2. Let $Q = \prod_{k=1}^{j}(X - y_k)$. If $j < n$, then since P_n is orthogonal to any polynomial of degree strictly lower than n, it holds that $\int QP_n w = 0$. However, by definition of Q, $P_n Q$ is non-negative, which leads to a contradiction.
3. Assume there exist nodes x_i and weights w_i such that the order of the method is $2n + 1$. Let $Z_{n+1} = \prod_{i=0}^{n}(X - x_i)$. Then for any polynomial function Q of degree equal or lower than n, the method is exact for any f of the form : $Z_{n+1}Q$. Thus :
$$\langle Z_{n+1}, Q\rangle = \sum_{k=0}^{n} w_i Z_{n+1}(x_i)Q(x_i) = 0$$
Z_{n+1} is thus orthogonal to all of $\mathbb{R}_n[X]$, therefore Z_{n+1} is proportional to the $n + 1$-th orthogonal polynomial P_{n+1}.
4. We have previously shown that the roots of any orthogonal polynomials are distinct. Therefore, since the nodes are roots of P_{n+1} they are unique. By taking functions f equal to the Lagrange basis with nodes x_i, one can easily show that : $w_i = \int_{\mathcal{X}} wL_i$. The weights are also uniquely defined.
5. Using the definition of Lagrange's basis L_i with the nodes x_i, define : $w_i = \int_{\mathcal{X}} L_i w$. Let $\mathcal{L}_n(f)$ be the Lagrange interpolation of f. For any polynomial function f of degree $\leq n$: it holds that $\int_{\mathcal{X}} fw = \int_{\mathcal{X}} \mathcal{L}_n(f)w = \sum_{i=0}^{n} f(x_i)\int_{\mathcal{X}} L_i w = \sum_{i=0}^{n} w_i f(x_i)$. Therefore, the order of the quadrature rule is at least n. Let's show that the order is $\geq 2n + 1$.

   Let $f \in \mathbb{R}_{2n+1}[X]$. Applying the Euclidean division of f by P_{n+1} leads to the existence of $Q, R \in \mathbb{R}_n[X]$ such that :
$$f = QP_{n+1} + R$$

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Therefore :

$$\int_{\mathcal{X}} wf = \int_{\mathcal{X}} QP_{n+1}w + \int_{\mathcal{X}} Rw \tag{1}$$
$$= \langle Q, P_{n+1} \rangle + \int_{\mathcal{X}} Rw \tag{2}$$
$$= \int_{\mathcal{X}} Rw \tag{3}$$

Where the last equality follows from the orthogonality of P_{n+1} over any polynomial in $\mathbb{R}_n[X]$. The integral of f is reduced to that of a polynomial of degree n at most. Since the order of the method is at least n :

$$\int_{\mathcal{X}} Rw = \sum_{i=0}^{n} w_i R(x_i)$$

.

However, $f(x_i) = Q(x_i)P_{n+1}(x_i) + R(x_i) = R(x_i)$ since $P_{n+1}(x_i) = 0$. Thus the quadrature is exact :

$$\int_{\mathcal{X}} wf = \sum_{i=0}^{n} w_i f(x_i)$$

.

6. Taking $f = P_{n+1}^2$ leads to a contradiction : null approximation but a positive integral.