



OPTIMAL QUADRATURE FORMULAS FOR FUNCTIONS WITH HIGHER-ORDER DERIVATIVES

Khazratkulov Sardor

Teacher at Academic Lyceum No. 2 of Karshi State Technical University

e-mail: hazratqulovsardor5@gmail.com

Abstract. This paper investigates the construction of optimal quadrature formulas for numerical integration of functions possessing higher-order derivatives. The study is formulated in Sobolev spaces and follows the Sard concept of optimality, in which the coefficients of a quadrature rule are chosen so as to minimize the norm of the associated error functional. A derivative-enriched quadrature model is considered on a uniform grid, and the exactness conditions, extremal error representation, and coefficient optimization problem are described. Special attention is paid to formulas obtained by supplementing nodal function values with odd-order derivatives at the endpoints. Such corrections lead to Euler–Maclaurin-type rules and substantially increase the algebraic order of accuracy for sufficiently smooth functions. A computational illustration for the integral of $\exp(x)$ on $[0,1]$ confirms the theoretical convergence behavior: the standard trapezoidal rule exhibits second-order convergence, the first-derivative corrected formula exhibits fourth-order convergence, and the formula containing both first- and third-derivative corrections exhibits sixth-order convergence. The results demonstrate that information on higher-order derivatives can be used systematically to reduce the norm of the integration error while preserving a simple grid structure. The presented approach is relevant to high-accuracy numerical integration, approximation theory, and the numerical solution of differential and integral equations.



Keywords: optimal quadrature formula; higher-order derivative; Sobolev space; Sard optimality; error functional; Euler–Maclaurin formula; numerical integration.

1. Introduction

Numerical integration is one of the fundamental operations of computational mathematics. Definite integrals arise in the discretization of differential equations, statistical estimation, mechanics, signal processing, computational physics, and many other applied problems. When an antiderivative is unavailable or inconvenient to evaluate, an integral is replaced by a weighted combination of function values, and possibly derivative values, at a finite set of nodes. The central problem is therefore not only to construct a quadrature formula, but also to choose its coefficients so that the approximation error is as small as possible on a prescribed class of functions.

The classical theory of optimal quadrature formulas is closely connected with the work of Sard and Sobolev. In Sard's formulation, the error of a quadrature formula is interpreted as a continuous linear functional on a normed function space, and a quadrature rule is called optimal if the norm of this error functional is minimal among all formulas of the chosen structural form. Sobolev subsequently developed a powerful functional-analytic and discrete-operator approach that makes it possible to derive explicit coefficients for broad families of optimal cubature and quadrature formulas. These ideas remain important because they provide a rigorous criterion of optimality rather than relying only on polynomial exactness or asymptotic order.

If the integrated function possesses derivatives of sufficiently high order, derivative data can be incorporated into the quadrature rule. This leads to formulas of Hermite, Euler–Maclaurin, and derivative-corrected types. The additional information is particularly useful when derivative values are already available from a differential equation, a spectral representation, an automatic differentiation



procedure, or a smooth numerical model. In such cases, higher-order derivatives can increase the convergence order without increasing the number of interior grid points.

Recent research continues to develop optimal formulas in Sobolev spaces, including formulas containing endpoint derivatives, positive-coefficient formulas, formulas for oscillatory integrals, and optimal integration rules in modified Sobolev spaces [1–8]. The present paper systematizes this framework for functions with higher-order derivatives and presents a compact IMRAD-style analysis of the construction principle, the corresponding error functional, and the convergence effect of derivative corrections.

The aim of the study is to formulate an optimal quadrature problem for smooth functions in a Sobolev setting, derive the structural conditions that determine the optimal coefficients, and numerically demonstrate how the use of higher-order derivatives improves the accuracy of integration. The principal hypothesis is that, for sufficiently smooth integrands, a derivative-enriched rule with optimally selected coefficients achieves a smaller error-functional norm and a higher convergence order than a rule based solely on function values.

2. Materials and Methods

2.1. Function space and quadrature model

Let $m \geq 1$ be an integer and let $W_2^{(m)}(0, 1)$ denote a Sobolev space of functions whose derivatives up to order $m-1$ are absolutely continuous in the appropriate sense and whose m -th derivative is square-integrable. For the seminorm-based formulation, the dominant smoothness measure is

$$\|f\|^2 = \int_0^1 |f^{(m)}(x)|^2 dx.$$

(1)

Consider a uniform grid $x_\beta = \beta h$, $\beta = 0, 1, \dots, N$, where $h = 1/N$. A general derivative-enriched quadrature formula can be represented as



$$\int_0^1 f(x) dx \approx \sum_{\beta=0}^{N-1} C_\beta f(x_\beta) + \sum_{j=1}^r [A_j f^{(2j-1)}(0) + B_j f^{(2j-1)}(1)], \quad (2)$$

where C_β are coefficients at the nodal function values and A_j, B_j are coefficients attached to endpoint derivatives. The highest derivative order used explicitly in the quadrature sum is $2r-1$, and the smoothness index m must be sufficiently large for all terms and the error functional to be well defined.

2.2. Error functional and Sard optimality

The error of formula (2) is written as the linear functional ℓ acting on f :

$$(\ell, f) = \int_0^1 f(x) dx - \sum_{\beta=0}^{N-1} C_\beta f(x_\beta) - \sum_{j=1}^r [A_j f^{(2j-1)}(0) + B_j f^{(2j-1)}(1)]. \quad (3)$$

For fixed nodes, the Sard problem consists in determining the coefficients that minimize the norm $\|\ell\|$ in the dual Sobolev space. In other words, the optimal coefficient vector C^* satisfies

$$\|\ell(C^*)\| = \min_C \|\ell(C)\|, \quad (4)$$

subject to the exactness constraints required by the null space of the Sobolev seminorm. For the classical seminorm generated by the m -th derivative, this normally requires annihilation of all polynomials of degree at most $m-1$ that lie in the kernel of the seminorm. Thus, moment conditions of the form

$$(\ell, x^k) = 0, \quad k=0, 1, \dots, m-1, \quad (5)$$

are imposed, with the derivative terms in (3) contributing to these conditions whenever k is sufficiently large. The constrained quadratic minimization problem obtained from (4) leads to a linear system for the unknown coefficients. In Sobolev's method, this system may be transformed by using a discrete analogue of the



differential operator d^{2m}/dx^{2m} . The resulting expressions typically contain roots of Euler–Frobenius polynomials with modulus less than one, which describe boundary-layer corrections to the interior weights.

2.3. Derivative corrections and Euler–Maclaurin structure

For a uniform mesh, a particularly transparent family is obtained from the Euler–Maclaurin expansion. Let $T_n(f)$ denote the composite trapezoidal rule. Then, for a sufficiently smooth function,

$$\int_0^1 f(x) dx = T_n(f) - \sum_{k=1}^r B_{2k} h^{2k}/(2k)! \cdot [f^{(2k-1)}(1) - f^{(2k-1)}(0)] + R_{2r}, \quad (6)$$

where B_{2k} are Bernoulli numbers and R_{2r} is the remainder. Keeping one correction term gives

$$Q_4(f) = T_n(f) - h^2/12 \cdot [f'(1) - f'(0)], \quad (7)$$

while keeping the first two odd-derivative corrections yields

$$Q_6(f) = T_n(f) - h^2/12 \cdot [f'(1) - f'(0)] + h^4/720 \cdot [f'''(1) - f'''(0)]. \quad (8)$$

The notation Q_4 and Q_6 emphasizes the expected fourth- and sixth-order behavior for smooth integrands. In the Sobolev optimality framework, formulas of this type arise naturally for particular smoothness classes. Previous studies have shown, for example, that Euler–Maclaurin-type rules are optimal in selected Sobolev spaces and that derivative-based optimal formulas can be obtained for arbitrary fixed N and appropriate m [2,3,6].

2.4. Computational experiment

To illustrate the theoretical effect of higher-order derivative information, the test integral $I = \int_0^1 \exp(x) dx = e - 1$ was evaluated on uniform meshes with $N = 4, 8, 16$,



and 32. Three formulas were compared: the composite trapezoidal rule T_n , the first-derivative corrected formula Q_4 in (7), and the first- plus third-derivative corrected formula Q_6 in (8). Since every derivative of $\exp(x)$ equals $\exp(x)$, the endpoint derivative differences are exactly $e-1$. Absolute errors were computed using the exact value $I = e-1$. This experiment is deterministic and reproducible and is intended to verify the asymptotic convergence rates rather than to serve as a statistical benchmark.

3. Results

3.1. Structural properties of the optimal rule

The minimization of the error-functional norm under the exactness constraints produces a symmetric coefficient system when the nodes are symmetric with respect to the midpoint of the interval. For a uniform grid on $[0,1]$, this implies $C_\beta = C_{N-\beta}$ for the function-value weights in the symmetric case. The interior coefficients approach their translation-invariant values as N increases, whereas corrections near the endpoints compensate for the boundary conditions inherent in the Sobolev extremal problem.

The principal theoretical effect of adding endpoint derivatives is the cancellation of leading terms in the asymptotic expansion of the quadrature error. The trapezoidal rule has a leading error proportional to $h^2[f'(1)-f'(0)]$. Subtracting the corresponding Bernoulli correction eliminates this term and shifts the leading contribution to order h^4 . Adding the third-derivative correction removes the h^4 term as well, making the next nonzero contribution of order h^6 . Therefore, under sufficient smoothness, the derivative-enriched formulas achieve higher accuracy without introducing additional interior nodes.

3.2. Numerical accuracy

Table 1 reports the absolute errors obtained for the exponential test function. The numerical values confirm the predicted hierarchy of convergence rates.



N	h	$ T_n - I $	$ Q_4 - I $	$ Q_6 - I $
4	0.250000	8.940076×10^{-3}	9.308425×10^{-6}	1.385079×10^{-8}
8	0.125000	2.236764×10^{-3}	5.824255×10^{-7}	2.166722×10^{-10}
16	0.062500	5.593001×10^{-4}	3.641175×10^{-8}	3.386846×10^{-12}
32	0.031250	1.398319×10^{-4}	2.275893×10^{-9}	5.306866×10^{-14}

Table 1. Absolute integration errors for $f(x) = \exp(x)$ on $[0, 1]$.

When the mesh width is halved, the trapezoidal error decreases by a factor close to 4, which is characteristic of second-order convergence. The error of Q_4 decreases by a factor close to 16, corresponding to fourth-order convergence. The error of Q_6 decreases by a factor close to 64 until floating-point round-off becomes noticeable, corresponding to sixth-order convergence. Thus the numerical experiment agrees with the cancellation mechanism in (6)–(8).

The observed orders p , estimated from consecutive errors by $p = \log_2(E_n/E_{2n})$, are summarized in Table 2.

Mesh refinement	T_n	Q_4	Q_6
$4 \rightarrow 8$	1.999	3.999	5.998
$8 \rightarrow 16$	2.000	4.000	5.999
$16 \rightarrow 32$	2.000	4.000	5.996*

Table 2. Observed convergence orders (*affected slightly by floating-point rounding).

4. Discussion

The results support the central premise of the study: higher-order derivative information can be converted into a substantial gain in quadrature accuracy. From the viewpoint of approximation theory, this gain occurs because the derivative terms enlarge the information set available to the quadrature functional. The coefficients can then be chosen to annihilate additional components of the integration error,



either through exactness conditions or through minimization of the dual norm in a Sobolev space.

The relationship between Sard optimality and Euler–Maclaurin corrections is particularly important. Polynomial exactness alone does not uniquely characterize an optimal formula in a normed space. Sard optimality instead asks for the smallest worst-case error over the unit ball of the chosen function space. In Sobolev spaces, this worst-case error is represented by the norm of the error functional, and the corresponding extremal function provides a rigorous measure of the remaining uncertainty. This interpretation explains why the choice of function space is not merely technical: changing the norm or the smoothness operator changes the geometry of the optimization problem and may lead to different optimal coefficients.

For practical computation, derivative-enhanced formulas are most attractive when derivative information is inexpensive. In the solution of boundary-value problems, for example, endpoint derivatives may already be part of the model. In automatic differentiation environments, high-order derivatives can sometimes be obtained with moderate additional cost. In spectral and symbolic computations, derivatives may be available analytically. Under these conditions, a fourth- or sixth-order corrected formula can outperform a lower-order formula on the same grid.

At the same time, the method has limitations. First, derivative values may be unavailable or contaminated by numerical noise. High-order numerical differentiation can amplify perturbations and may eliminate the theoretical advantage of the formula. Second, the Sobolev smoothness assumptions must be satisfied; if the integrand has weak regularity, discontinuities, endpoint singularities, or rapidly varying local behavior, the expected convergence order may not be realized. Third, an optimal formula for one function space need not be optimal for another. Therefore, the term “optimal” must always be interpreted relative to the specified class of functions, norm, nodes, and information functionals.



The computational example uses an analytic function and therefore represents a best-case smooth regime. Nevertheless, the measured orders are useful because they directly confirm the asymptotic structure predicted by the theory. Future work can extend the experiment to nonuniform grids, weighted integrals, oscillatory kernels, complex-valued Sobolev spaces, multidimensional cubature, and numerical tests in which derivative data are perturbed. Another relevant direction is the automatic selection of the derivative order according to a cost-versus-accuracy criterion.

5. Conclusion

An optimal-quadrature framework for functions with higher-order derivatives has been presented in a Sobolev-space setting. The quadrature error was formulated as a continuous linear functional, and Sard optimality was defined through minimization of its dual norm under exactness constraints. This approach provides a rigorous mechanism for determining optimal coefficients rather than relying exclusively on heuristic corrections.

Derivative-enriched formulas based on endpoint odd-order derivatives were then considered. The Euler–Maclaurin representation shows that the first-derivative correction cancels the leading $O(h^2)$ term of the trapezoidal error, while the additional third-derivative correction cancels the $O(h^4)$ term. The numerical experiment for $\exp(x)$ confirmed convergence orders of approximately 2, 4, and 6 for the trapezoidal, first-derivative corrected, and first-plus-third-derivative corrected formulas, respectively.

Consequently, for sufficiently smooth functions and reliably available derivative data, optimal quadrature formulas with higher-order derivatives provide a computationally efficient route to high-accuracy integration. Their effectiveness is especially pronounced when increasing the number of nodes is expensive but derivative information is already accessible. The Sobolev–Sard framework remains



a natural theoretical foundation for extending these formulas to more general integration problems.

References

- [1] Sard, A. (1949). Best approximate integration formulas; best approximation formulas. American Journal of Mathematics, 71(1), 80–91. <https://doi.org/10.2307/2372095>
- [2] Sard, A. (1963). Linear Approximation. American Mathematical Society, Providence.
- [3] Sobolev, S. L. (1974). Introduction to the Theory of Cubature Formulas. Nauka, Moscow. [In Russian].
- [4] Nikolsky, S. M. (1988). Quadrature Formulas. Nauka, Moscow. [In Russian].
- [5] Sobolev, S. L., & Vaskevich, V. L. (1996). Cubature Formulas. Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk. [In Russian].
- [6] Shadimetov, K. M., Hayotov, A. R., & Nuraliev, F. A. (2013). On an optimal quadrature formula in Sobolev space $L_2^{(m)}(0,1)$. Journal of Computational and Applied Mathematics, 243, 91–112. <https://doi.org/10.1016/j.cam.2012.11.010>
- [7] Shadimetov, K. M., & Hayotov, A. R. (2014). Optimal quadrature formulas in the sense of Sard in $W_2^{(m,m-1)}$ space. Calcolo, 51, 211–243. <https://doi.org/10.1007/s10092-013-0076-6>
- [8] Shadimetov, K. M., & Nuraliev, F. A. (2018). Optimal formulas of numerical integration with derivatives in Sobolev space. Journal of Siberian Federal University. Mathematics & Physics, 11(6), 764–775. <https://doi.org/10.17516/1997-1397-2018-11-6-764-775>



- [9] Shadimetov, K. M., Tursunmurodov, S. T. (2025). Optimal quadrature formulas in the Sobolev space of complex-valued functions. *Uzbek Mathematical Journal*, 69(4), 194–200. <https://doi.org/10.29229/uzmj.2025-4-19>
- [10] Shadimetov, K. M., Adilkhodjaev, A., & Gulomov, O. (2025). Optimal quadrature formulas for approximate calculation of rapidly oscillating integrals. *Results in Applied Mathematics*, 27, 100627. <https://doi.org/10.1016/j.rinam.2025.100627>