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NUMERICAL INTEGRATION BY USING LOCAL–NODE GAUSS–HERMITE CUBATURE

R. D. Millán, A. M. Rosolen and M. Arroyo*

LaCàN, Universitat Politècnica de Catalunya,
C/Jordi Girona 1-3, Barcelona 08934, Spain.
e-mail: daniel.millan,adrian.rosolen,marino.arroyo@upc.edu
web: http://www-lacan.upc.es

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Abstract. *A local–node numerical integration scheme for meshless methods is presented in this work. The distinguishing characteristic of the introduced scheme is that not support mesh or grid to perform numerical integration is needed, besides the fact that gauss cubature points for each node are generated in a properly fashion and that the extension of the methodology to high dimensions is straightforward. The numerical integration is computed with the Gauss–Hermite cubature formulas, and the partition of unity is employed to introduce the Gaussian weight in a natural way. Selected numerical tests in two-dimensions are used to illustrate the validity of the proposed methodology. Although the obtained results are encouraging, the behavior of the integration error is not still well understood when the dimensionless parameter which control the width of the Gaussian kernel varies.*

1 INTRODUCTION

Gaussian quadratures are used to approximate the integral of a function $f(\mathbf{x})$ over a specified domain $\Omega \in \mathbb{R}^d$ by using a known weighting kernel $\psi(\mathbf{x})$. The concept of quadrature is similar to that of numerical integration, especially when they are referred to one-dimensional integrals. Although the term quadrature is also applied for higher dimensional integration, two- and higher-dimensional integration are actually called cubature.

In one dimension, an n-point quadrature rule can exactly evaluate the integral of a polynomial of order up to $2n-1$. Therefore, if the function $f(x)$ is well approximated by a polynomial of order $m = 2n-1$, then a quadrature with n *quadrature points* or *nodes* suffices for a good estimate of the integral, i.e.

$$I(f) = \int_\Omega f(x)\psi(x)dx \approx \sum_{i=1}^{n} w_i f(x_i). \tag{1}$$

The nodes x_i and weights w_i are uniquely determined by the choice of the domain Ω and the weighting kernel $\psi(x)$. In fact, one may go as far as to say that the choice of the domain and the kernel defines a quadrature. In particular, the location of the nodes x_i are given by the roots of the polynomial of order m in the sequence of orthonormal polynomials $\{\pi_j\}$ generated by the metric $\langle \pi_j, \pi_k \rangle := \int_\Omega \pi_j(x)\pi_k(x)\psi(x)dx = \delta_{jk}$, and the weights w_i can be computed from a linear system once the roots are known. The mathematics of quadrature methods is well understood and described in most textbooks on numerical analysis[8].

1.1 Contrasts Between One Variable and More Than One Variable. Extracted from [8]

The theory of integration formulas like Equation (1) for functions of one variable is well developed. A great deal of this theory can be found in the books by Krylov[6], Davis and Rabinowitz[3], and Stroud and Secrest[9]. Formulas for the Equation (1) are relatively easy to construct and, unless $f(x)$ is badly behaved. There is not difficulty in obtaining an accurate approximation to the integral. The reason this is true is related to the following two facts:

1. One-dimensional space is much simpler geometrically than two- or higher-dimensional spaces. Since all finite line segments are equivalent under an affine transformation there is essentially only one bounded connected region in E_1.

2. The theory of integration formulas is closely connected with the theory of orthogonal polynomials. In one variable the theory of orthogonal polynomials is fairly simple and fairly completely known and is of great use in the construction of formulas.

Here E_d denotes real d-dimensional Euclidean space.

Although quite a number of integration formulas for multiple integrals are known the theory of such formulas is far from complete. This is due largely to the greater complexity of E_d, which can be summarized in part as follows:

- For each $d \geq 2$ there are infinitely many distinct, bounded connected regions in E_d. In E_2, for example, the square, circle, and triangle are tree regions which are not equivalent under an affine transformation. Integration formulas for any one of these regions are different from formulas for the others.

- The theory of orthogonal polynomials is more complicated in more than one variable. No formulas have seen constructed in d-dimensions, $d \geq 3$, using the theory of orthogonal polynomials in d variables.

1.2 Product Formulas and Stability

In most cases d one-dimensional formulas, each of degree m, are combined to give a formula of degree m for $\mathbb{R}^d$. These deterministic cubature rules commonly are cited as

the standard tensor product cubature formulas. Thus, in multiple dimensions the computation of the above integral, Equation (1), if an n-point integration rule is used in each dimension in a d-dimensional space, needs n^d function evaluations. The computational burden therefore increases significantly with dimension d. This is often referred as the *curse of dimensionality*.

In order to avoid the so-called curse of dimensionality, specific cubature rules are made to approximate the numerical integration by taking into account the particularities of the domains and the weight functions. For the interested reader, we commend the paper of Cools [2], a very nice survey on this matter.

Another important issue that arises when an integration rule is used concerns with its stability factor. Generally speaking from the perspective of integration, a rule with all its points inside the integration region and all its weights positive is more desirable and will have a small error than a formula for which one or both of these properties is lacking [8]. Integration rules with both positive and negative weights are particularly undesirable if the magnitude of the weights are large compared with $I(1)$. The reason is that a large amount of roundoff error is introduced if

$$\sum_{i=1}^{n} |w_i| \gg \sum_{i=1}^{n} w_i = I(1).$$

Therefore, a standard measure of the stability factor of an integration rule is the ratio between the sum of the absolute values of the weights and $I(1)$, $C = \sum_{i=1}^{n} |w_i|/I(1)$ [4]. A completely stable rule has $C = 1$, but so far there is no known general method for constructing stable but efficient rules. For example the product Gauss–Hermite rule do have $C = 1$, but the number n^d of the f values needed for a degree $2n - 1$ product Gauss–Hermite rule grows so rapidly with n that using this rules becomes infeasible for practical calculations when $d > 3$ or 4.

1.3 Gauss-Hermite Cubature

In this work, we are interested in to analyse numerical schemes which contain Gaussian weight factors. The Gauss-Hermite cubature rules are the most appropriate to take into account such factors.

In the case of multiple integrals over infinite regions $\mathbb{R}^d$, and with integration kernel given by $e^{-|\mathbf{x}|^2}$, the associate cubature scheme is known commonly under the name of Gauss-Hermite since in one-dimension the involved orthogonal polynomials turn out to be Hermite polynomials. Also Gauss-Hermite cubature is of fundamental importance in many areas of applied mathematics that uses statistical representations, i.e. applied sciences, financial mathematics, statistics and actuarial sciences[4, 7]. For this cubature rule we have $I(1) = \pi^{d/2}$ [8].

Reliable routines for the calculation of the roots and weights are readily available and most mathematical software packages provide means for one-dimensional Gauss-Hermite

quadrature calculations [10]. For higher dimensions, there are not any free software package available, and rules are tabulated only for specific cases [8, 4].

The structure of the paper is as follows. In Section 2, the methodology is described. In Section 3, selected numerical examples are shown. Some concluding remarks and future work are finally indicated in Section 4.

2 Methods

Let $X = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\} \subset \mathbb{R}^d$ be a set of points sampling a domain Ω embedded in $\mathbb{R}^d$, and $f(\mathbf{x})$ a scalar function defined in Ω. The goal is to compute the numerical integral of $f(\mathbf{x})$ in Ω.

A local neighborhood of $\mathbf{x}$ is defined in terms of a weighting function ϕ, following the maximum entropy philosophy, we use a Gaussian weight[1]:

$$\phi(|\mathbf{x} - \mathbf{x}_a|) = \exp(-\beta|\mathbf{x} - \mathbf{x}_a|^2).$$

In numerical applications, this weight behaves like a compactly supported weight. For efficiency, we thus define the neighbor index set of $\mathbf{x}$ as

$$\mathcal{N}^{\mathbf{x}} = \{a \in \{1, 2, ..., N\} \mid \phi(|\mathbf{x} - \mathbf{x}_a|) > \texttt{TOL}\}.$$

Although explicitly not noted, the parameter β may be a function of $\mathbf{x}$. It sets the range of these hat functions, which should be large enough to reach enough neighbors.

2.1 Partition Of Unity

The first step in the method is to define a partition of unity based on the point set. For instance, consider Shepard's shape functions based on Gaussian weights:

$$q_a(\mathbf{x}) = \frac{\exp(-\beta_a|\mathbf{x} - \mathbf{x}_a|^2)}{\sum_{b\in N^{\mathbf{x}}} \exp(-\beta_b|\mathbf{x} - \mathbf{x}_b|^2)} = \frac{\exp(-\beta_a|\mathbf{x} - \mathbf{x}_a|^2)}{Z(\mathbf{x})}, \quad \mathbf{x} \in \Omega, \tag{2}$$

although any other non-negative and smooth weighting function could be used. The parameter β_a sets the range of these hat functions, and depends on the local point density.

Following, the partition of unity is applied to the integration of a scalar function $f(x)$ in a domain Ω:

$$
\begin{aligned}
\int_\Omega f(\mathbf{x})d\mathbf{x} &= \int_\Omega 1\, f(\mathbf{x})d\mathbf{x} \\
&= \int_\Omega \left(\sum_{a\in N^{\mathbf{x}}} q_a(\mathbf{x})\right) f(\mathbf{x})d\mathbf{x} \\
&= \sum_{a=1}^{N} \int_\Omega q_a(\mathbf{x})\ f(\mathbf{x})d\mathbf{x} \\
&= \sum_{a=1}^{N} \int_\Omega \frac{f(\mathbf{x})}{Z(\mathbf{x})} e^{\beta_a|\mathbf{x}-\mathbf{x}_a|^2} d\mathbf{x},
\end{aligned}
\tag{3}
$$

Substituting $\mathbf{x} = \mathbf{x}_a + \boldsymbol{\xi}/\beta_a^{d/2}$, the Equation (3) becomes:

$$
\begin{aligned}
\int_\Omega f(\mathbf{x})d\mathbf{x} &= \sum_{a=1}^{N} \int_\Omega \frac{f(\boldsymbol{\xi})}{\beta_a^{d/2} Z(\boldsymbol{\xi})} e^{|\boldsymbol{\xi}|^2} d\boldsymbol{\xi} \\
&\approx \sum_{a=1}^{N} \sum_{i=1}^{n} \frac{w(\mathbf{x}_i) f(\mathbf{x}_i)}{\beta_a^{d/2} Z(\mathbf{x}_i)}.
\end{aligned}
\tag{4}
$$

3 Results

The proposed methodology is examined in 5 test functions, which are shown in Equations (5)–(9).

$$f_1(\mathbf{x}) = e^{-\zeta|\mathbf{x}-\mathbf{x}^*|^2} \tag{5}$$

$$f_2(\mathbf{x}) = \left[\prod_{i=1}^{d} g(x_i)\right] e^{-\zeta|\mathbf{x}-\mathbf{x}^*|^2} \tag{6}$$

$$f_3(\mathbf{x}) = \sqrt{\zeta}\left[\prod_{i=1}^{d} (1-g(x_i))\right] e^{-\zeta|\mathbf{x}-\mathbf{x}^*|^2} \tag{7}$$

$$f_4(\mathbf{x}) = \left[\prod_{i=1}^{d} (1-2g(x_i))\right] e^{-\zeta|\mathbf{x}-\mathbf{x}^*|^2} \tag{8}$$

$$f_5(\mathbf{x}) = \zeta|\mathbf{x}-\mathbf{x}^*|^2 e^{-\zeta|\mathbf{x}-\mathbf{x}^*|^2} \tag{9}$$

where $g(x_i) = \cos(5\pi(x_i - x_i^*))$, such that $i = 1, 2, \ldots, d$. These functions are shown when $d = 2$ in Figure 1, where it can be seen that the parameter ζ is chosen such that the $f_i(\mathbf{x})$ vanish on the boundary. This is done in order to avoid no desirable boundary effects.

The analytical integration of those functions was obtained by using `Mathematica`. It is important to remark that this work is only focus on the case $d = 2$.

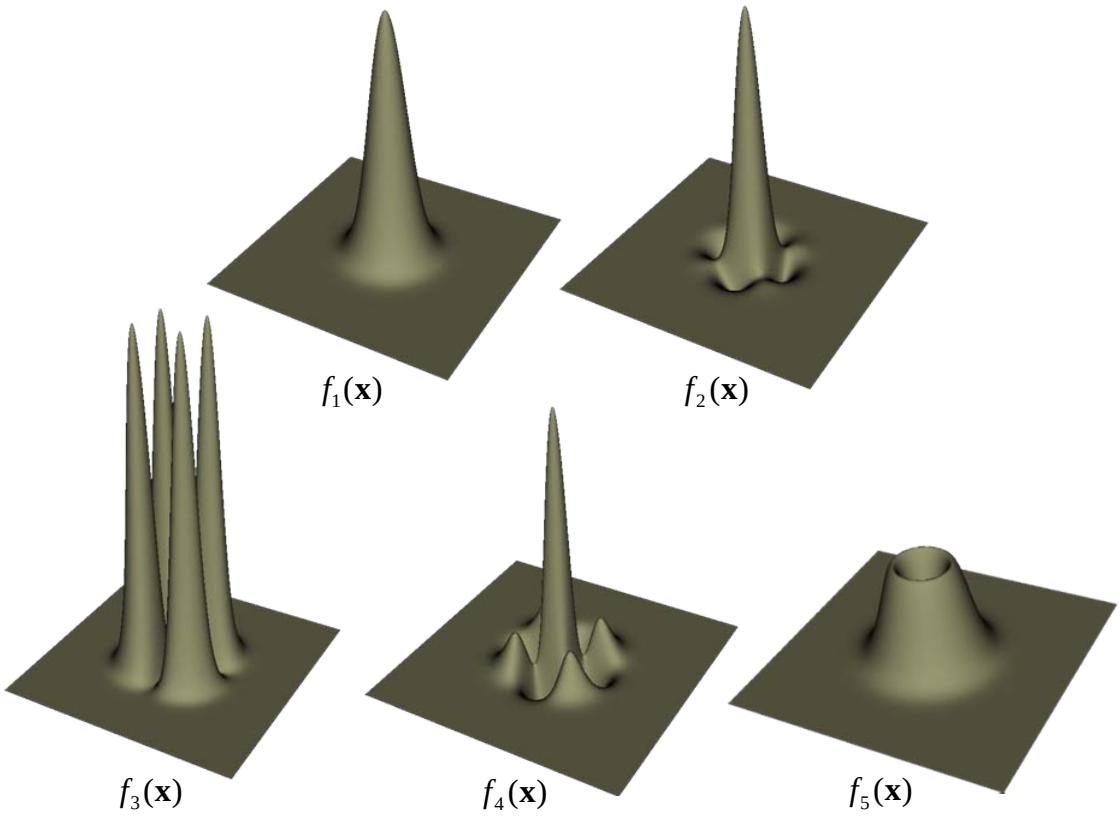


Figure 1: Test functions used to analyse the proposed numerical integration methodology with $\zeta = 100$. Note that the ζ parameter is chosen such that the $f_i(\mathbf{x})$ vanish on the boundary of $\Omega = [0,1] \times [0,1]$.

Figure 2 shows the integration error as a function of the dimensionless parameter $\gamma = \beta h^2$ for a two-dimensional node set, $n = 10$ sample points (order $m = 6$) for each node were used [5]. The value of h is a measurement of the nodal spacing, and $\beta_a = \beta = \gamma/h^2$ is constant over the domain $\Omega = [0,1] \times [0,1]$, $a = 1, \ldots, N$. Therefore, the shape functions locality degree is controlled by the parameter γ. Finally, also are presented the results for computing Gauss-Legendre numerical integration rule with $n = 12$ gauss points for each triangle (order $m = 7$).

The integration error as a function of the parameter γ is depicted in Figure 3 for the expressions $f_3(\mathbf{x})$ and $f_4(\mathbf{x})$, which respectively present the worst and the best performance in the Figure 2. The illustrated results corresponds to three sets of two-dimensional nodes, $h = 1/16, 1/32, 1/64$.

4 DISCUSSIONS AND CONCLUSIONS

In this paper, an efficient and novel d-dimensional numerical integration scheme based on partition of unity and Gauss-Hermite cubature rule is presented. The aim of the

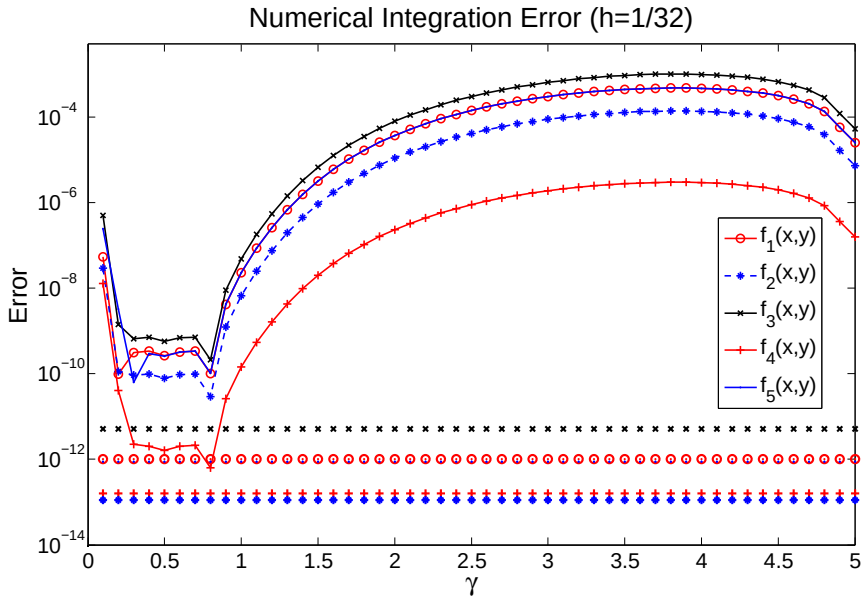
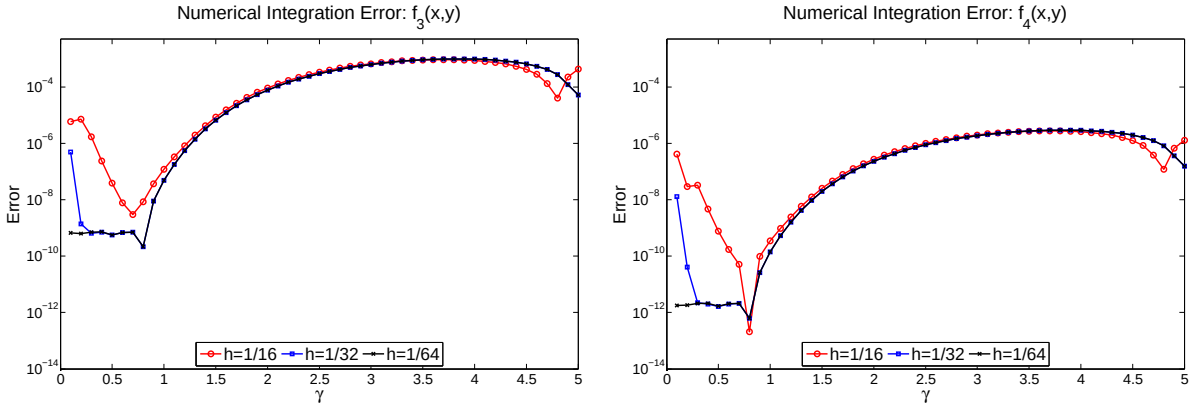


Figure 2: Numerical integration error for the Equations (5)–(9) when the parameter γ varies int the range [0.1, 5]. The horizontal curves (without lines) correspond to the Gauss-Legendre cubature, while the others are obtained by the approximation based on Gauss-Hermite cubature. It was used a structured mesh of hexagonal elements with $h = 1/32$.



(a) (b)

Figure 3: Integration error for the functions that present the worst (a) and the best (b) performance in Figure 2. Three sets of two-dimensional nodes ($h = 1/16, 1/32, 1/64$) were used.

proposed methodology is to deal with problems in which no support mesh or any other structured relationship for the node set is prescribed. The main drawback in the formulation is related with the treatment of the nodes closest to the boundary, because they

contribute with sample points outside of the domain. In particular, we noted that the value of $I(1)$ is not satisfied when a pruning to delete the sample points external to the domain is performed. For this reason, 5 test functions which vanish close to the boundary were analysed in order to assess the methodology. Regardless the encouraging results obtained for some values of γ, disappoint the fact that the integration error behavior is not still well understood when this dimensionless parameter which control the width of the Gaussian kernel varies.

We believe that the main causes of the results behavior is related (1) with the partition of unity or (2) with a possible conceptual error in the formulation. In summary, no concluding assessment of the methodology can be done, and it is necessary to perform more studies.

We are currently working on a mixed formulation by merging Gauss-Legendre and Gauss-Hermite integration rules to avoid boundary effects. The idea is to apply the first one to the closest boundary nodes while the second one is used for the rest.

Future lines of research involve the extension of the formulation for a non Euclidean tensor metric, and the validation of the approach to solve PDE's with numerical meshfree schemes.

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