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On the identification of symmetric quadrature rules for finite element methods

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ABSTRACT

In this paper we describe a methodology for the identification of symmetric quadrature rules inside of quadrilaterals, triangles, tetrahedra, prisms, pyramids, and hexahedra. The methodology is free from manual intervention and is capable of identifying a set of rules with a given strength and a given number of points. We also present *polyquad* which is an implementation of our methodology. Using polyquad v1.0 we proceed to derive a complete set of symmetric rules on the aforementioned domains. All rules possess purely positive weights and have all points inside the domain. Many of the rules appear to be new, and an improvement over those tabulated in the literature.

1. Introduction

When using the finite element method to solve a system of partial differential equations it is often necessary to evaluate surface and volume integrals inside of a standardised domain $\mathbf{\Omega}$ [1–3]. A popular numerical integration technique is that of Gaussian quadrature in which

$$\int_{\mathbf{\Omega}} f(\mathbf{x})\,\mathrm{d}\mathbf{x} \approx \sum_{i}^{N_p} \omega_i f(\mathbf{x}_i), \tag{1}$$

where $f(\mathbf{x})$ is the function to be integrated, $\{\mathbf{x}_i\}$ are a set of N_p points, and $\{\omega_i\}$ the set of associated weights. The points and weights are said to define a *quadrature rule*. A rule is said to be of strength ϕ if it is capable of exactly integrating any polynomial of maximal degree ϕ over $\mathbf{\Omega}$. A degree ϕ polynomial $p(\mathbf{x})$ with $\mathbf{x} \in \mathbf{\Omega}$ can be expressed as a linear combination of basis polynomials

$$p(\mathbf{x}) = \sum_{i}^{|\mathscr{P}^\phi|} \alpha_i \mathscr{P}_i^\phi(\mathbf{x}), \quad \alpha_i = \int_{\mathbf{\Omega}} p(\mathbf{x}) \mathscr{P}_i^\phi(\mathbf{x})\,\mathrm{d}\mathbf{x}, \tag{2}$$

where $\mathscr{P}^\phi$ is the set of basis polynomials of degree $\leq \phi$ whose cardinality is given by $|\mathscr{P}^\phi|$. From the linearity of integration it therefore follows that a strength ϕ quadrature rule is one which can exactly integrate the basis. Taking $f \in \mathscr{P}^\phi$ the task of obtaining an N_p point quadrature rule of strength ϕ is hence reduced to finding a solution to a system of $|\mathscr{P}^\phi|$ nonlinear equations. This system can be seen to possess $(N_D + 1)N_p$ degrees of freedom where $N_D \geq 2$ corresponds to the number of spatial dimensions.

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In the case of $N_p \lesssim 10$ the above system can often be solved analytically using a computer algebra package. However, beyond this it is usually necessary to solve the above system – or a simplification thereof – numerically. Much of the research into multidimensional quadrature over the past five decades has been directed towards the development of such numerical methods. The traditional objective when constructing quadrature rules is to obtain a rule of strength ϕ inside of a domain $\mathbf{\Omega}$ using the fewest number of points. To this end efficient quadrature rules have been derived for a variety of domains: triangles [4–13], quadrilaterals [11,14,15], tetrahedra [7,9,16,17], prisms [18], pyramids [19], and hexahedra [11,20–22]. For finite element applications it is desirable that (i) points are arranged symmetrically inside of the domain, (ii) all of the points are strictly inside of the domain, and (iii) all of the weights are positive. The consideration given to these criteria in the literature cited above depends strongly on the intended field of application—not all rules are derived with finite element methods in mind.

Much of the existing literature is predicated on the assumption that the integrand sits in the space of $\mathcal{P}^{\phi}$. Under this assumption there is little, other than the criteria listed above, to distinguish two N_p rules of strength ϕ; both can be expected to compute the integral exactly with the same number of functional evaluations. It is therefore common practice to terminate the rule discovery process as soon as a rule is found. However, there are cases when either the integrand is inherently non-polynomial in nature, e.g. the quotient of two polynomials, or of a high degree, e.g. a polynomial raised to a high power. In these circumstances the above assumption no longer holds and it is necessary to consider the truncation term associated with each rule. Hence, within this context it is no longer clear that the traditional objective of minimising the number of points required to obtain a rule of given strength is suitable: it is possible that the addition of an extra point will permit the integration of several of the basis functions of degree $\phi + 1$.

Over the past five or so years there has also been an increased interest in numerical schemes where the same set of points are used for both integration and interpolation. One example of such a scheme is the flux reconstruction (FR) approach introduced by Huynh [23]. In the FR approach there is a need for quadrature rules that (i) are symmetric, (ii) remain strictly inside of the domain, (iii) have a prescribed number of points, and (iv) are associated with a well conditioned nodal basis for polynomial interpolation. These last two requirements exclude many of the points tabulated in the literature. Consequently, there is a need for *bespoke* or *designer* quadrature rules with non-standard properties.

This paper describes a methodology for the derivation of symmetric quadrature rules inside of a variety of computational domains. The method accepts both the number of points and the desired quadrature strength as free parameters and – if successful – yields a set of rules. Traits, such as the positivity of the weights, can then be assessed and rules binned according to their suitability for various applications. The remainder of this paper is structured as follows. In Section 2 we introduce the six reference domains and enumerate their symmetries. Our methodology is presented in Section 3. Based on the approach of Witherden and Vincent [12] the methodology requires no manual intervention and avoids issues relating to ill-conditioning. In Section 4 we proceed to describe our open-source implementation, *polyquad*. Using polyquad a variety of truncation-optimised rules, many of which appear to improve over those tabulated in the literature, are obtained and presented in Section 5. Finally, conclusions are drawn in Section 6.

2. Bases, symmetries, and domains

2.1. Basis polynomials

The defining property of a quadrature rule for a domain $\mathbf{\Omega}$ is its ability to exactly integrate the set of basis polynomials, $\mathcal{P}^{\phi}$. This set has an infinite number of representations the simplest of which being the monomials. In two dimensions we can express the monomials as

$$\mathcal{P}^{\phi} = \left\{ x^i y^j \mid 0 \le i \le \phi,\ 0 \le j \le \phi - i \right\}, \tag{3}$$

where ϕ is the maximal degree. Unfortunately, at higher degrees the monomials become extremely sensitive to small perturbations in the inputs. This gives rise to polynomial systems which are poorly conditioned and hence difficult to solve numerically [9,16]. A solution to this is to switch to an *orthonormal basis set* defined in two dimensions as

$$\mathcal{P}^{\phi} = \left\{ \psi_{ij}(\mathbf{x}) \mid 0 \le i \le \phi,\ 0 \le j \le \phi - i \right\}, \tag{4}$$

where $\mathbf{x} = (x, y)^T$ and $\psi_{ij}(\mathbf{x})$ satisfies $\forall \mu, \nu$

$$\int_{\mathbf{\Omega}} \psi_{ij}(\mathbf{x}) \psi_{\mu\nu}(\mathbf{x})\, \mathrm{d}\mathbf{x} = \delta_{i\mu}\delta_{j\nu}, \tag{5}$$

where $\delta_{i\mu}$ is the Kronecker delta. In addition to being exceptionally well conditioned orthonormal polynomial bases have other useful properties. Taking the constant mode of the basis to be $\psi_{00}(\mathbf{x}) = 1/c$ we see that

$$\int_{\mathbf{\Omega}} \psi_{ij}(\mathbf{x})\, \mathrm{d}\mathbf{x} = c \int_{\mathbf{\Omega}} \psi_{00}(\mathbf{x}) \psi_{ij}(\mathbf{x})\, \mathrm{d}\mathbf{x} = c\delta_{i0}\delta_{j0}, \tag{6}$$