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Stable high-order quadrature rules with equidistant points

Daan Huybrechs [*,1]

Department of Computer Science, Katholieke Universiteit Leuven, Belgium

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ABSTRACT

Newton–Cotes quadrature rules are based on polynomial interpolation in a set of equidistant points. They are very useful in applications where sampled function values are only available on a regular grid. Yet, these rules rapidly become unstable for high orders. In this paper we review two techniques to construct stable high-order quadrature rules using equidistant quadrature points. The stability follows from the fact that all coefficients are positive. This result can be achieved by allowing the number of quadrature points to be larger than the polynomial order of accuracy. The computed approximations then implicitly correspond to the integral of a least squares approximation of the integrand. We show how the underlying discrete least squares approximation can be optimised for the purpose of numerical integration.

1. Introduction

A recurring problem in computational science is the approximate evaluation of the integral

$$I[f] := \int_a^b w(x)f(x)\,\mathrm{d}x \approx Q[f] := \sum_{j=1}^{N} w_j f(x_j) \tag{1}$$

by a quadrature $Q[f]$ rule with N points x_i and weights w_i. There is a rich body of literature on numerical integration; we refer the reader to the volumes [1–5] and the references therein for a broad overview.

A case of great practical importance is that where f is known only in equidistant points, i.e., in the points

$$x_j = a + (j-1)\frac{b-a}{N-1}, \quad j = 1, \ldots, N, \tag{2}$$

with $N \geq 2$. Equidistant points often arise in finite difference methods and collocation methods for ordinary and partial differential equations [6,7] or integral equations [8]. Popular quadrature rules in this setting are the (composite) trapezoidal rule and Simpson rules. These are low-order variants of the family of Newton–Cotes rules, which for the set of N points (2) are exact for all polynomials up to degree at least $N-1$. Newton–Cotes rules are easy to apply and easy to implement for a variety of weight functions $w(x)$, but the low-order rules converge slowly and the high-order rules are numerically unstable. We will discuss these properties in more detail in Section 2.

* Tel.: +32 16 327829; fax: +32 16 327996.
E-mail address: daan.huybrechs@cs.kuleuven.be.

1 The author is a Postdoctoral Fellow of the Research Foundation — Flanders (FWO).

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Stability in numerical integration follows from having positive weights. It is well known that quadrature rules with positive weights converge for all continuous functions f on $[a, b]$. An important issue in numerical integration is therefore the construction of quadrature rules of a certain order d with positive weights. We say that a quadrature rule has order d if it is exact for all polynomials up to degree $d - 1$. A fundamental theorem in numerical integration, due originally to Tchakaloff [9], states that suitable rules exist with only d quadrature points:

Proposition 1.1. *For any functional $I[f]$ of the form (1) with a positive weight function $w(x) > 0$, and for any integer $d > 0$, a quadrature rule of order d exists with d points and with all weights positive.*

When searching for rules with positive weights, Tchakaloff's result supplies an upper bound on the required number of points. The theorem is more general than stated here and holds for a variety of basis functions and for higher dimensions (see, e.g., the introduction of [10] for a full statement of the theorem). For the case of polynomials and univariate integrals, the problem of determining such rules is completely resolved by the existence of Gaussian quadrature and Clenshaw–Curtis quadrature. These rules however do not have equidistant points. The problem in higher dimensions is much more challenging [11].

It turns out that rules with positive weights can be constructed on equidistant grids by letting the number of quadrature points N be larger than the order d of the rule. This is possible for any order d, as long as N is sufficiently large. It follows that such rules may have $N \gg d$ nonzero weights. However, in that case another quadrature rule of the same order exists on the same grid with only d weights, that are all positive:

Proposition 1.2. *If a quadrature rule of order d exists for $I[f]$ with $N \geq d$ points and with positive weights, then a quadrature rule of order d exists for $I[f]$ with the same points but with only d nonzero weights, all positive.*

This result is due to Davis [10], based on earlier results in [12]. We may conclude that, if N is sufficiently large, a rule on the equidistant grid exists that achieves Tchakaloff's upper bound. The growth of N for increasing order d was later established in [13]:

Proposition 1.3. *Let N be the minimal number of quadrature points such that a quadrature rule of order d with positive weights exists on the equidistant grid (2). It is true that*

$$N \sim d^2, \quad d \gg 1.$$

The minimal number of points N grows as Cd^2. The constant C is fairly modest in practice. We will illustrate numerically in this paper that $C \approx 0.07$ for the case $w(x) = 1$. This means, for example, that a quadrature rule of order 20 requires only $N = 33$. Conversely, when samples are given on an equidistant grid with N points, a quadrature rule of order $d \approx \frac{1}{0.07}\sqrt{N}$ with positive weights may be used to integrate the function.

A first technique to construct quadrature rules with positive coefficients is by solving a least squares problem. The connection between quadrature rules and discrete least squares problems was also examined in [14]. It appears that this connection has not been further explored in a systematic manner since the publication in 1970 of [14,13]. On the other hand it has long been, and still is, quite common to construct a (discrete) least squares approximation of a (sampled) function. This approximation can then be integrated exactly. We intend to show in this paper that the link between least squares approximations and quadrature rules does have advantages. First, the requirement that the weights should be positive yields a natural and generally applicable stopping criterion for discrete least squares approximations. Increasing the degree beyond a certain value may yield numerical instability for certain functions. Second, the connection with least squares problems supplies a numerically stable and efficient way to construct quadrature rules with positive weights on sets of equidistant or arbitrarily spaced points. Explicit expressions for the weights can easily be derived in terms of discrete orthogonal polynomials. Third, discrete least squares approximations for the sole purpose of numerical integration benefit from optimised choices of a weighted discrete inner product. The weight factors themselves are related to quadrature rules with positive weights.

A second technique to construct quadrature rules with positive coefficients is by looking for quadrature rules predicted to exist by Proposition 1.2. The construction of a quadrature rule with only d positive weights, corresponding to d out of N possible equidistant points, can be achieved by solving a least squares problem subject to linear inequality constraints. A convergent algorithm for this particular type of problem was proposed in [15] and called the NNLS algorithm (nonnegative least squares). The result is a class of interpolatory quadrature rules with guaranteed numerical stability and convergence for increasing order.

We continue the paper in Section 2 with an illustration of the difficulties of using Newton–Cotes quadrature. We describe least squares quadrature rules in Section 3, a stable implementation based on the method of Forsythe in Section 4 and nonnegative least squares methods in Section 5. We end the paper with numerical results in Section 6.

We would like to stress the fact that most of the theory in Section 2 is present already in the papers [14,13]. In this paper, we supplement a self-contained description of this theory with pointers to and descriptions of applicable existing algorithms and with extensive numerical examples in the later sections.