Journal of Computational and Applied Mathematics 296 (2016) 709–723

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Gaussian quadrature for splines via homotopy continuation: Rules for C^2 cubic splines

Michael Bartoň [a,*], Victor Manuel Calo [a,b]

[a] Numerical Porous Media Center, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia

[b] Applied Mathematics & Computational Science and Earth Science & Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia

A R T I C L E I N F O

Article history:
Received 17 May 2015
Received in revised form 20 August 2015

Keywords:
Gaussian quadrature
B-splines
Well-constrained polynomial system
Polynomial homotopy continuation

A B S T R A C T

We introduce a new concept for generating optimal quadrature rules for splines. To generate an optimal quadrature rule in a given (target) spline space, we build an associated source space with known optimal quadrature and transfer the rule from the source space to the target one, while preserving the number of quadrature points and therefore optimality. The quadrature nodes and weights are, considered as a higher-dimensional point, a zero of a particular system of polynomial equations. As the space is continuously deformed by changing the source knot vector, the quadrature rule gets updated using polynomial homotopy continuation. For example, starting with C^1 cubic splines with uniform knot sequences, we demonstrate the methodology by deriving the optimal rules for uniform C^2 cubic spline spaces where the rule was only conjectured to date. We validate our algorithm by showing that the resulting quadrature rule is independent of the path chosen between the target and the source knot vectors as well as the source rule chosen.

1. Introduction

Numerical integration of univariate functions is a fundamental mathematical task which is a subroutine of many complex algorithms and is typically frequently invoked. Naturally, such an integration (or quadrature) rule must be as efficient as possible. We derive a new class of quadrature rules that are optimal in the sense that they require the minimum number of function's evaluations.

A quadrature rule, or in short a *quadrature*, is an *m-point rule*, if m evaluations of a function f are needed to approximate its weighted integral over a closed interval $[a, b]$

$$\int_a^b w(x) f(x)\, \mathrm{d}x = \sum_{i=1}^{m} \omega_i f(\tau_i) + R_m(f), \tag{1}$$

where w is a fixed non-negative *weight function* defined over $[a, b]$. The rule is required to be *exact*, that is, $R_m(f) \equiv 0$ for each element of a predefined linear function space $\mathcal{L}$. The rule is said to be *optimal* if m is the minimum number of *weights* ω_i and *nodes* τ_i; in this case, nodes are points at which f is evaluated.

* Corresponding author.
E-mail addresses: Michael.Barton@kaust.edu.sa (M. Bartoň), Victor.Calo@kaust.edu.sa (V.M. Calo).

http://dx.doi.org/10.1016/j.cam.2015.09.036

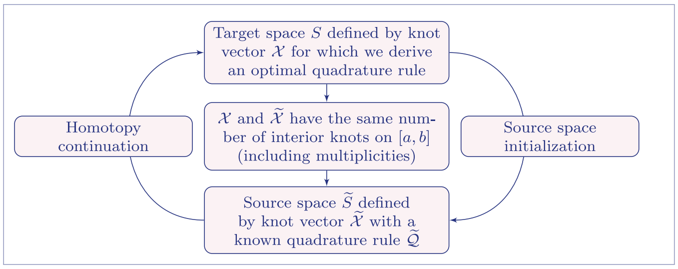

Fig. 1. Spline space initialization flowchart.

For the space of polynomials, the optimal rule is known to be the classical Gaussian quadrature [1] with the order of exactness $2m - 1$, that is, only m evaluations are needed to exactly integrate any polynomial of degree at most $2m - 1$. Consider a sequence of polynomials $(p_0, p_1, \ldots, p_m, \ldots)$ that form an orthogonal basis with respect to the scalar product

$$\langle f, g \rangle = \int_a^b f(x) g(x) w(x) \mathrm{d}x. \tag{2}$$

The quadrature points are the roots of the mth orthogonal polynomial p_m which in the case when $w(x) \equiv 1$ is the degree-m Legendre polynomial [2].

In this paper, we focus on piece-wise cubic polynomials, i.e., cubic splines, but the methodology is general and could be used for higher degrees as well. A univariate space of cubic splines is uniquely determined by its *knot vector*. This knot vector is a non-decreasing sequence of real numbers called *knots*, and the multiplicity of each knot determines the smoothness between the cubic pieces. To simplify the argument, we first study uniform knot vectors with all interior knots with *uniform multiplicity*. In particular, we investigate knot vectors with single interior knots which yield C^2 cubic splines and knot vectors with double interior knots which give C^1 cubic splines. For a more detailed introduction on splines, we refer the reader to [3–5].

The quadrature rules for splines have been studied since the late 50s [6–9]. Firstly conjectured by Schoenberg [6] and later proved by Micchelli and Pinkus [8], the conditions of the existence and uniqueness of the optimal (Gaussian) rule have been derived. For spline spaces with maximum continuity (e.g., C^2 cubic splines), Micchelli and Pinkus [8] proved that a *unique* Gaussian quadrature rule always exists. Their result, moreover, also reveals a nice phenomenon: the number of optimal nodes stays fixed as long as the number of interior knots stays constant. Therefore if one desires to derive a class of quadrature rules with the same number of nodes, spline spaces with higher continuity must have adequately more subintervals (elements) than spaces of lower continuity. This is natural because splines of lower continuity are limits of those of higher continuity, when merging continuously two (or several) knots together, and their result is in agreement with this fact.

For spaces with lower continuity, or when boundary constraints are involved, the rule is not guaranteed to be unique. Only spaces with fixed continuities were studied in [8]. To the best of our knowledge, the results on existence and uniqueness are not known for spaces built above knot vectors with mixed continuities; we refer to these as knot vectors with mixed multiplicities. For example, for cubic splines, this includes knot vectors with both single and double knots. In this work, we derive quadratures for this kind of mixed continuity spaces and show numerically that optimal quadratures exist.

We use the observation that one spline space with multiple knots is a limit case of another spline space with the same number of single knots (when counting the multiplicities) when two, or several, knots merge. Abstracting this merging as a continuous transition between the two knot vectors of the same cardinality, the *source* and the *target* ones, we continuously evolve the corresponding spline spaces from one into the other. The quadrature rule also depends *continuously* on the spline space since the quadrature rule can be seen as a zero (root) of a certain polynomial system and an infinitesimal change of the system does not significantly change the root. Based on these facts, we propose a new methodology that for a given (target) spline space S generates an associated source space $\widetilde{S}$ where the Gaussian quadrature rule is known. These spaces are generated above knot vectors $\mathcal{X}$ and $\widetilde{\mathcal{X}}$, respectively, and the quadrature rule $\widetilde{\mathcal{Q}}$ of $\widetilde{S}$ is numerically traced as $\widetilde{\mathcal{X}}$ evolves into $\mathcal{X}$, see Fig. 1.

The rest of the paper is organized as follows. Section 2 briefly overviews the homotopy continuation of polynomial systems and Section 3 summarizes a few basic properties of cubic splines. In Section 4, we introduce a homotopy-continuation-based algorithm, and in Section 5, we discuss the results and the validity of the new quadratures obtained. Finally, in Section 6, we summarize our conclusions and describe the directions for future research.

2. Homotopy continuation for polynomial systems

Polynomial homotopy continuation (PHC) is a numerical scheme that solves polynomial systems of equations. This approach was introduced to solve the problem of movability of kinematic mechanisms [10] where the variables are the free parameters of a certain mechanism tied together by a set of polynomial constraints. However, the unknowns and the