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Commuting extensions and cubature formulae

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Abstract Based on a novel point of view on 1-dimensional Gaussian quadrature, we present a new approach to d-dimensional cubature formulae. It is well known that the nodes of 1-dimensional Gaussian quadrature can be computed as eigenvalues of the so-called Jacobi matrix. The d-dimensional analog is that cubature nodes can be obtained from the eigenvalues of certain mutually commuting matrices. These are obtained by extending (adding rows and columns to) certain non-commuting matrices $A_1, \ldots, A_d$, related to the coordinate operators $x_1, \ldots, x_d$, in $\mathbf{R}^d$. We prove a correspondence between cubature formulae and "commuting extensions" of $A_1, \ldots, A_d$, satisfying a compatibility condition which, in appropriate coordinates, constrains certain blocks in the extended matrices to be zero. Thus, the problem of finding cubature formulae can be transformed to the problem of computing (and then simultaneously diagonalizing) commuting extensions. We give a general discussion of existence and of the expected size of commuting extensions and briefly describe our attempts at computing them.

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1 Introduction

One of the most elegant topics in numerical analysis is the theory of Gaussian quadrature [7]. Unfortunately this theory is limited to one dimension, and although

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something is known about generalizations to multiple dimensions (see [3] for a survey article and many references), at the moment there are many more questions than answers. The aim of this paper is to present a new approach to cubature rules ("cubature" seems to be the name given to the generalization of quadrature to arbitrary dimension). In classical, one-dimensional Gaussian quadrature, the most widely used method for computing cubature nodes and weights, developed about 35 years ago [11], involves solving the eigenproblem for a certain tridiagonal matrix (see [15] for a recent "basis independent" discussion of this). Our proposed method for computing d-dimensional cubature formulae involves the construction of d matrices (with tridiagonal block structure in suitable bases), extending these, in a manner we will explain below, to a set of commuting matrices, and then solving the simultaneous eigenproblem for these commuting matrices. An important step in this process, which follows very naturally from a new approach we present to one-dimensional Gaussian quadrature, is the need to construct *commuting extensions* of a set of matrices. We say the $N \times N$ matrices $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ are $N \times N$ commuting extensions of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$ (here $N \geq n$) if the top left $n \times n$ block in $\tilde{A}_i$ is A_i, for each $i = 1, 2, \ldots, d$, and the matrices $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ pairwise commute.

The idea of commuting extensions is very natural, but we do not find any such notion in the linear algebra or numerical linear algebra literature. Since we hope this idea will find other applications, the first few sections in this paper explore the subject without reference to cubature rules. Section 2 covers basic theory and briefly mentions a couple of simple algorithms for computing commuting extensions, with which we currently have very limited success. Section 3 discusses commuting extensions when the matrices A_i take a special form, relevant for the study of cubature rules.

In section 4 we turn to the theory of cubature rules. Subsection 4.1 contains a novel approach to one dimensional Gaussian quadrature, based upon the properties of a certain operator, its eigenvalues and eigenfunctions. This serves as the model for all the subsequent discussion. In subsection 4.2 we consider the natural extension of this approach to multiple dimensions, and prove the central results of the paper, giving an equivalence between odd degree, positive weight cubature rules and commuting extensions (satisying a compatibility condition that will be explained in the sequel) of a certain set of matrices. Subsection 4.3 includes some simple consequences of this relationship. One of the key results in the theory of cubature rules, a lower bound on the number of nodes needed for an odd degree cubature rule, originating in the work of Möller [13], follows from a general result in the theory of commuting extensions (theorem 2). Similarly a simple result on the spectra of commuting extensions (theorem 6) gives interesting constraints on the nodes in positive weight cubature rules, which we believe have hitherto been overlooked even in one dimension. Section 4.3 also briefly mentions our attempts to actually apply the commuting extension approach for computing nodes and weights. Our achievements are rather limited, nevertheless they validate our approach, and even give a few new cubature formulae. Section 5 contains a list of open questions.

In the final stages of preparing this manuscript we learned that the connection between cubature nodes and common eigenvalues of commuting extensions has been noticed by Y. Xu. Xu's observations appear in a much wider discussion connecting cubature nodes with zeros of quasi-orthogonal multivariable polynomials [20], [23]. It seems however that the possibility of constructing cubature formulae via commuting extensions has been largely ignored by scientists working in this field. Apart from bringing this approach to the attention of a broader audience and proposing it as a potentially valuable tool to compute new formulae, our work presents a novel and exceedingly simple proof of the correspondence between cubature nodes and joint eigenvalues of commuting extensions.

We close this introduction by mentioning that one of the oldest continuing applications of Gaussian quadrature is in quantum mechanics, where it is used, in the so-called "DVR method" for the computation of matrix elements of non-exactly solvable Hamiltonians (see [10] for early references and [16] for recent reviews). This paper was born out of an attempt to extend the DVR method to higher dimensions; other, recent progress on this subject has been made by Dawes and Carrington [8]. Another interesting perspective on DVR can be found in the paper [12].

2 Commuting Extensions

In this section we present the basic theory of commuting extensions.

Definition 1 *We say the $N \times N$ matrices $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ are $N \times N$* commuting extensions *of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$ (here $N \geq n$) if the top left $n \times n$ block in $\tilde{A}_i$ is A_i, for each $i = 1, 2, \ldots, d$, and the matrices $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ pairwise commute.*

Theorem 1 *Any set of matrices admits commuting extensions.*

Proof We construct explicit commuting extensions of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$. Take

$$\tilde{A}_1 = \begin{pmatrix} A_1 & A_2 & A_3 & \ldots & A_d \\ A_d & A_1 & A_2 & \ldots & A_{d-1} \\ A_{d-1} & A_d & A_1 & \ldots & A_{d-2} \\ \vdots & \vdots & \vdots & & \vdots \\ A_2 & A_3 & A_4 & \ldots & A_1 \end{pmatrix}, \quad \tilde{A}_2 = \begin{pmatrix} A_2 & A_3 & A_4 & \ldots & A_1 \\ A_1 & A_2 & A_3 & \ldots & A_d \\ A_d & A_1 & A_2 & \ldots & A_{d-1} \\ \vdots & \vdots & \vdots & & \vdots \\ A_3 & A_4 & A_5 & \ldots & A_2 \end{pmatrix}, \quad \text{etc.} \tag{1}$$

Such matrices are known as "block circulants"; in [6] it is proven that block circulants commute. □

Theorem 1 establishes the existence of commuting extensions, but it is natural to ask what is the smallest possible dimension for commuting extensions of a given set of matrices. To this end we have the following result:

Theorem 2 *If $N \times N$ commuting extensions of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$ exist, then*

$$N \geq n + \frac{1}{2}\max_{i,j}\text{rank}([A_i, A_j]) \, . \tag{2}$$

Proof Suppose $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ are $N \times N$ commuting extensions of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$. Write

$$\tilde{A}_i = \begin{pmatrix} A_i & a_i \\ b_i & \alpha_i \end{pmatrix}, \tag{3}$$

where the matrices a_i, b_i, α_i have sizes $n \times (N-n)$, $(N-n) \times n$, $(N-n) \times (N-n)$ respectively. The top left $n \times n$ block of the equation $[\tilde{A}_i, \tilde{A}_j] = 0$ gives the requirement

$$[A_i, A_j] + a_i b_j - a_j b_i = 0 . \tag{4}$$

Since the matrices a_i and b_i do not have rank exceeding $(N-n)$, neither do products of the form $a_i b_j$, and the matrices $a_i b_j - a_j b_i$ can have rank at most $2(N-n)$. Thus (4) can hold only if for each i, j we have

$$\operatorname{rank}([A_i, A_j]) \leq 2(N-n) , \tag{5}$$

and the theorem follows directly. □

Unfortunately there is a large gap between the lower bound on N from theorem 2 and the N in the existence proof of theorem 1. In practice, it seems that the lower bound of theorem 2 is rarely attained, and the N of theorem 1 is much too big. As we shall see in section 4, theorem 2 gives rise to a well known lower bound on the number of points needed for a cubature formula, and in that context also the bound can rarely be attained.

In addition to not knowing, in general, any way to rigorously predict the lowest dimension for commuting extensions of a given set of matrices, we also currently have no way of determining how many distinct families of commuting extensions of a given dimension exist. By a family we mean a set of commuting extensions related by conjugation as described in the following obvious result:

Theorem 3 *If the matrices $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$ are $N \times N$ commuting extensions of the $n \times n$ matrices $A_1, A_2, \ldots, A_d$, then so are the matrices $\tilde{U}\tilde{A}_1\tilde{U}^{-1}, \tilde{U}\tilde{A}_2\tilde{U}^{-1}, \ldots, \tilde{U}\tilde{A}_d\tilde{U}^{-1}$, where $\tilde{U}$ is any matrix of the form*

$$\tilde{U} = \begin{pmatrix} I_{n \times n} & 0_{n \times (N-n)} \\ 0_{(N-n) \times n} & U \end{pmatrix} \tag{6}$$

with U an invertible $(N-n) \times (N-n)$ matrix.

To proceed further, and at least get some idea of the size needed for commuting extensions, we have to resort to parameter counting. From here on we restrict to the case where the matrices A_i and $\tilde{A}_i$ are symmetric, i.e. the case of symmetric *commuting extensions of a set of* symmetric *matrices. Note that except when $d = 2$ the existence construction of theorem 1 does not guarantee symmetric commuting extensions. Neither is it clear that the lowest dimension commuting extensions of* *a set of symmetric matrices need necessarily be symmetric. But because the case of symmetric commuting extensions of symmetric matrices is relevant for cubature rules, we restrict our attention to this.*

If the matrices $\tilde{A}_i$ are symmetric then we can write

$$\tilde{A}_i = \begin{pmatrix} A_i & a_i \\ a_i^T & \alpha_i \end{pmatrix} \tag{7}$$

where a_i is $n \times (N-n)$ and α_i is $(N-n) \times (N-n)$ and symmetric. Thus the number of free parameters we have in choosing the extensions of the A_i is

$$d\left(n(N-n) + \frac{1}{2}(N-n)(N-n+1)\right) = \frac{1}{2}d(N-n)(N+n+1) \; . \tag{8}$$

Let us assume that at least one of the $\tilde{A}_i$, say $\tilde{A}_1$, has distinct eigenvalues. Then all matrices that commute with $\tilde{A}_1$ also commute amongst themselves, and we just need to check that $[\tilde{A}_1, \tilde{A}_i] = 0$ for $i = 2, \ldots, d$. Since the commutator of symmetric matrices is automatically antisymmetric, we have

$$\frac{1}{2}N(N-1)(d-1) \tag{9}$$

equations to satisfy. We cannot, however, directly compare the number of parameters from (8) *with the number of equations from* (9)*, as from theorem 3 we learn that (except when $N = n+1$) commuting extensions exist in families. For symmetric commuting extensions the matrices U (and thus $\tilde{U}$) in theorem 3 are restricted to be orthogonal. So symmetric commuting extensions occur in families with $\frac{1}{2}(N-n)(N-n-1)$ parameters, and the number of parameters in choosing extensions should exceed the number of equations from* (9) *by at least this amount. Thus we need*

$$\frac{1}{2}d(N-n)(N+n+1) \geq \frac{1}{2}N(N-1)(d-1) + \frac{1}{2}(N-n)(N-n-1) \; . \tag{10}$$

A little rearranging of this inequality gives the condition

$$N - n \geq \frac{n(n-1)(d-1)}{2(n+d)} = \frac{d-1}{2}n - \frac{d^2-1}{2} + \frac{d(d^2-1)}{2n} + o\left(\frac{1}{n}\right) \; , \tag{11}$$

where the $o\left(\frac{1}{n}\right)$ term is equal to $\frac{d^2(1-d^2)}{2n(d+n)}$. If N satisfies this condition we expect to find $N \times N$ symmetric commuting extensions. For comparison, in the explicit commuting extensions of theorem 1 (which, however, were not symmetric) we had $N - n = (d-1)n$; we can clearly expect to do much better than this.

On occasions it seems that parameter counting can be misleading. As an example consider the case of $d = 2$. From theorem 2 we have $N - n \geq \frac{1}{2}\mathrm{rank}([A_1, A_2])$ (note that since the commutator of two symmetric matrices is antisymmetric, its rank is always even). The parameter counting argument tells us that we should expect

$$N - n \geq \frac{n(n-1)}{2(n+2)} \; . \tag{12}$$

Assuming $[A_1, A_2]$ *of maximal rank we have*

$$\frac{1}{2}\text{rank}([A_1, A_2]) = \begin{pmatrix} \frac{n}{2} & n \text{ even} \\ \frac{n-1}{2} & n \text{ odd} \end{pmatrix}. \tag{13}$$

So by theorem 2

$$N - n \geq \begin{pmatrix} \frac{n}{2} & n \text{ even} \\ \frac{n-1}{2} & n \text{ odd} \end{pmatrix}. \tag{14}$$

We see that when $d = 2$ *and* $[A_1, A_2]$ *is of maximal rank the inequality from parameter counting is actually weaker than the rigorous one from theorem 2. Thus in this case the parameter counting argument is certainly flawed. But this seems to be rather exceptional; in general it appears that when it is consistent with the lower bound of theorem 2, parameter counting gives a better idea of the size we should expect for commuting extensions. In particular the following theorem holds.*

Theorem 4 *For* $n > 5$ *there exist symmetric* $n \times n$ *matrices* A_1, A_2 *with* rank $([A_1, A_2]) = 2$ *and no* $(n+1) \times (n+1)$ *symmetric commuting extensions.*

The technical details of the proof are omitted. For such matrices the lower bound of theorem 2 can not be attained, at least with symmetric extensions.

Note on index conventions: In discussion of commuting extensions we start with d matrices of size $n \times n$ which we extend to size $N \times N$. For clarity, in most of this paper we adhere to the following index conventions:

Indices i, j, k etc. run from 1 to d.
Indices a, b, c etc. run from 1 to n
Indices α, β, γ etc. run from 1 to N.

The results up to here all concern the existence and size of commuting extensions. For the purpose of finding commuting extensions we will use the following:

Theorem 5 *The* $n \times n$ *symmetric matrices* $A_1, A_2, \ldots, A_d$ *admit* $N \times N$ *symmetric commuting extensions if and only if there exist* $N \times N$ *diagonal matrices* $\Lambda_1, \Lambda_2, \ldots, \Lambda_d$ *and an* $n \times N$ *matrix* Q *with orthonormal rows such that*

$$A_i = Q \Lambda_i Q^T \ . \tag{15}$$

Proof *From the extensions to* Λ_i, Q*:* If we can find $N \times N$ symmetric commuting extensions $\tilde{A}_1, \tilde{A}_2, \ldots, \tilde{A}_d$, then we can find diagonal matrices $\Lambda_1, \Lambda_2, \ldots, \Lambda_d$ and an $N \times N$ orthogonal matrix $\tilde{Q}$ such that

$$\tilde{A}_i = \tilde{Q} \Lambda_i \tilde{Q}^T \ . \tag{16}$$

The matrix Q in the theorem is comprised of just the first n rows of $\tilde{Q}$.

From Λ_i, Q *to the extensions:* A matrix Q as described in the theorem can always be extended, by the addition of $N - n$ orthonormal rows, to an $N \times N$ orthogonal matrix $\tilde{Q}$. (In fact this can be done in many ways, corresponding to the freedom described in Theorem 3.) Once $\tilde{Q}$ has been constructed the matrices $\tilde{A}_i = \tilde{Q} \Lambda_i \tilde{Q}^T$ are $N \times N$ symmetric commuting extensions of the A_i. □

Note The matrix Q in theorem 5 satisfies $QQ^T = I_{n\times n}$.

It is of interest to understand how the spectra of commuting extensions (i.e. the entries of the matrices Λ_i in Theorem 5) are related to the spectra of the original matrices A_i. The following is a first result in this direction. It is a simple consequence of the Sturmian separation theorem [18], but we offer a direct proof too.

Theorem 6 *Let $\tilde{A}$ be an $N \times N$ symmetric extension of the $n \times n$ (symmetric) matrix A. Then the smallest eigenvalue of $\tilde{A}$ is less than or equal to the smallest eigenvalue of A, and the largest eigenvalue of $\tilde{A}$ is greater than or equal to the largest eigenvalue of A.*

Proof It is well known that for any $m \times m$ symmetric matrix M the smallest and largest eigenvalues are given by

$$\min_{x\neq 0} \frac{x^T M x}{x^T x}, \qquad \max_{x\neq 0} \frac{x^T M x}{x^T x}, \tag{17}$$

respectively, where x is a vector with m entries. The proof follows then from the following inequalities

$$\min_{x\neq 0} \frac{x^T \tilde{A} x}{x^T x} \leq \min_{y\neq 0} \frac{y^T A y}{y^T y}, \qquad \max_{x\neq 0} \frac{x^T \tilde{A} x}{x^T x} \geq \max_{y\neq 0} \frac{y^T A y}{y^T y}. \tag{18}$$

□

We now briefly discuss our attempts to compute commuting extensions. The most obvious approach is simply to treat the unknown entries in the extended matrices $\tilde{A}_i$ as variables, and to consider the conditions $[\tilde{A}_i, \tilde{A}_j] = 0$ as equations in these variables. In the generic case (generically we should expect the $\tilde{A}_i$ to have distinct eigenvalues) it will be sufficient to look at the equations just for one particular value of i. If $N - n > 1$, then by theorem 3 we expect continuous families of extensions, this freedom can be exploited to fix some of the variables. The system of equations we obtain will be quadratic in the unknown variables. We have done some initial experiments with this approach in the case $d = 2$, attempting to solve the system of quadratic equations 1) by integrating the gradient flow $v' = -\nabla||[\tilde{A}_1(v), \tilde{A}_2(v)]||^2$ (here v denotes the variables added to form the commuting extensions), and 2) using Newton's method. The results are very varied; for some pairs of moderate-sized matrices there is reasonable convergence, but in other cases there are signs of extreme ill-conditioning (very low gradients in the case of gradient flow, almost singular Jacobian in Newton's method). Some of the cubature related results mentioned in the sequel were obtained by integration of the gradient flow with Frobenius norm of the commutator; a detailed description of these calculations can be found in [9]. Another approach we have tried for finding the $\tilde{A}_i$ uses successive Jacobi rotations applied to $\tilde{Q}$ together with an appropriate update of $\{\Lambda_i\}$ so that in each step $S = \sum_{i=1}^{d} \|A_i - Q\Lambda_i Q^T\|^2$ is minimized ($\tilde{Q},\ Q,\ \Lambda$ are as in theorem 5). This method also exhibits severe slowing down for large A_i.

It is clear from our results that a lot more work is necessary on the topic of computing commuting extensions.

3 A Special Case Of Commuting Extensions

We turn to consideration of a special case of commuting extensions that turns out to be relevant for cubature formula. It is characterized by 2 conditions: First, the symmetric $n \times n$ matrices A_i for which we wish to find commuting extensions are block tridiagonal

$$A_i = \begin{pmatrix} \alpha_{i1} & a_{i1} & 0 & \dots & 0 & 0 \\ a_{i1}^T & \alpha_{i2} & a_{i2} & \dots & 0 & 0 \\ 0 & a_{i2}^T & \alpha_{i3} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \alpha_{i(r-1)} & a_{i(r-1)} \\ 0 & 0 & 0 & \dots & a_{i(r-1)}^T & \alpha_{ir} \end{pmatrix}. \tag{19}$$

Here $\alpha_{i1}, \alpha_{i2}, \dots, \alpha_{ir}$ are symmetric square matrices of sizes $n_1 \times n_1, n_2 \times n_2, \dots, n_r \times n_r$ respectively, where $n_1 + n_2 + \dots + n_r = n$. The matrices $a_{i1}, a_{i2}, \dots, a_{i(r-1)}$ are of size $n_1 \times n_2, n_2 \times n_3, \dots, n_{r-1} \times n_r$ respectively. The second condition we impose is that the commutator matrices $[A_i, A_j]$ all vanish except for a single block in the bottom right hand corner, of size $n_r \times n_r$.

Let us seek symmetric commuting extensions with the matrices $\tilde{A}_i$, of size $N \times N$, also taking tridiagonal block form, that is

$$\tilde{A}_i = \begin{pmatrix} \alpha_{i1} & a_{i1} & 0 & \dots & 0 & 0 & 0 \\ a_{i1}^T & \alpha_{i2} & a_{i2} & \dots & 0 & 0 & 0 \\ 0 & a_{i2}^T & \alpha_{i3} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \alpha_{i(r-1)} & a_{i(r-1)} & 0 \\ 0 & 0 & 0 & \dots & a_{i(r-1)}^T & \alpha_{ir} & a_i \\ 0 & 0 & 0 & \dots & 0 & a_i^T & \alpha_i \end{pmatrix}, \tag{20}$$

where the new blocks α_i are of size $(N-n) \times (N-n)$ and are symmetric, and the a_i are of size $n_r \times (N-n)$.

The questions we wish to ask are (1) what are the equations that the new blocks α_i, a_i have to satisfy? and (2) how large need N be for us to have a hope that such extensions exist? As in section 2, we assume that $\tilde{A}_1$ has distinct eigenvalues, so we need only check that $\tilde{A}_1$ commutes with the $d-1$ matrices $\tilde{A}_2, \dots, \tilde{A}_d$ and this guarantees that all the $\tilde{A}_i$ mutually commute. A brief calculation, using the fact that the commutators $[A_1, A_i]$ are zero except for a single block, gives the following conditions:

$$\left.\begin{aligned} a_{1(r-1)}a_i - a_{i(r-1)}a_1 &= 0 \\ a_{1(r-1)}^T a_{i(r-1)} - a_{i(r-1)}^T a_{1(r-1)} + \alpha_{1r}\alpha_{ir} - \alpha_{ir}\alpha_{1r} + a_1 a_i^T - a_i a_1^T &= 0 \\ \alpha_{1r}a_i - \alpha_{ir}a_1 + a_1\alpha_i - a_i\alpha_1 &= 0 \\ a_1^T a_i - a_i^T a_1 + \alpha_1\alpha_i - \alpha_i\alpha_1 &= 0 \end{aligned}\right\} \quad i = 2, \dots, d\,. \tag{21}$$

Of these four equations for each i, the first is of size $n_{r-1} \times (N-n)$, the second is of size $n_r \times n_r$ and antisymmetric, the third is of size $n_r \times (N-n)$ and the fourth is of size $(N-n) \times (N-n)$ and antisymmetric. Thus there is a total of

$$(d-1)\ \left(n_{r-1}(N-n) + \frac{1}{2}n_r(n_r-1) \right.$$
$$\left. + n_r(N-n) + \frac{1}{2}(N-n)(N-n-1)\right) \tag{22}$$

equations to be satisfied. The number of variables available in the a_i and α_i is

$$d\left(n_r(N-n) + \frac{1}{2}(N-n)(N-n+1)\right)\ . \tag{23}$$

The system of equations (21), has an invariance

$$a_i \to a_i g\ , \qquad \alpha_i \to g^T \alpha_i g\ , \qquad i = 1, \ldots, r \tag{24}$$

where g is an $(N-n) \times (N-n)$ orthogonal matrix. Thus it is not sufficient that the number of variables simply exceed the number of equations to be solved, it must exceed the number of equations to be solved by at least $\frac{1}{2}(N-n)(N-n-1)$ to give a full family of solutions. Thus we can expect solutions provided:

$$d\left(n_r(N-n) + \frac{1}{2}(N-n)(N-n+1)\right) \geq \frac{1}{2}(N-n)(N-n-1)$$
$$+(d-1)\left(n_{r-1}(N-n) + \frac{1}{2}n_r(n_r-1)\right.$$
$$\left. + n_r(N-n) + \frac{1}{2}(N-n)(N-n-1)\right) \tag{25}$$

Simplifying this gives

$$N - n \geq \frac{n_r(n_r-1)}{2\left(\frac{n_r+d}{d-1} - n_{r-1}\right)}\ , \tag{26}$$

where we have made the assumption that the denominator on the right hand side is positive.

Note the right hand side in (26) does not depend on the total dimension, n, of the matrices A_i, but just on n_{r-1} and n_r. Thus the size of the extensions needed in this special case may well be substantially smaller than in general. The application to cubature of this special form of commuting extensions will become clear in section 4.3.

4 Cubature Formulae and Commuting Extensions

Much of the contents of this section, with some additions, are also discussed in [9]. In section 4.1 we give a novel presentation on the subject of Gaussian quadrature; in section 4.2 this is extended to the case of multidimensional cubature. Section 4.3 discusses some practical aspects and consequences of the results of 4.2.

4.1 A Novel Approach to Gaussian Quadrature

In Gaussian quadrature we wish to find $q+1$ nodes $x_0, \dots, x_q$ and $q+1$ weights $w_0, \dots, w_q$ such that the quadrature rule

$$\int_\Omega w(x) f(x) dx \approx \sum_{i=0}^{q} w_i f(x_i) \tag{27}$$

is exact whenever $f(x)$ is a polynomial of degree at most $2q+1$. Here Ω is some interval or union of intervals and $w(x) \geq 0$ is a suitable weight function. *Throughout this paper we only consider quadrature and cubature rules with positive weights, i.e. $w_i > 0$.*

Note In this subsection there is no mention of commuting extensions so we allow ourselves to break our index conventions. In this subsection alone indices i, j, k run from 0 to q.

Denote by $\mathcal{P}_q$ the space of polynomials of degree at most q with the inner product

$$\langle a|b\rangle = \int_\Omega w(x) a(x) b(x) dx \ , \qquad \forall a, b \in \mathcal{P}_q \ . \tag{28}$$

Let Π_q be the projector from $\mathcal{P}_{q+1}$ onto $\mathcal{P}_q$ parallel to its orthogonal complement $\mathcal{P}_q^\perp$ *i.e.* the obvious orthogonal projection onto $\mathcal{P}_q$ with respect to the inner product above. We define the operator $\chi : \mathcal{P}_q \to \mathcal{P}_q$ by $\chi p = \Pi_q x p$ for all $p \in \mathcal{P}_q$. Since χ is self adjoint there is an orthonormal basis of $\mathcal{P}_q$ consisting of eigenfunctions $\{u_i\}$ of χ, $\chi u_i = \Lambda_i u_i$. Associated with χ there is a symmetric bilinear form X on $\mathcal{P}_q$ defined by $X(a, b) = \langle a|\chi b\rangle$, or equivalently

$$X(a, b) = \int_\Omega w(x) a(x) x b(x) \, dx \ , \qquad \forall a, b \in \mathcal{P}_q \ . \tag{29}$$

X is diagonalised in the basis $\{u_i\}$, $X(u_i, u_j) = \Lambda_i \delta_{ij}$.

We prove below that the eigenvalues $\{\Lambda_i\}$ of χ provide nodes for a Gaussian quadrature formula of degree $2q+1$. Our treatment is the reverse of the classical presentation of Gaussian quadrature [7], [11], see the explanation after theorem 8.

We need the following remarkable lemma:

Lemma 1 *(The δ lemma) Let p be an arbitrary polynomial in $\mathcal{P}_{q+1}$. Then*

$$\langle p|u_i\rangle = \langle 1|u_i\rangle p(\Lambda_i) \ , \tag{30}$$

i.e. the inner product of p with u_i is determined, up to normalization, by evaluation of p at Λ_i.

Note In this lemma p is allowed to be in $\mathcal{P}_{q+1}$.

Proof We prove recursively for j that

$$\langle x^j|u_i\rangle = \langle 1|u_i\rangle \Lambda_i^j \ , \qquad j = 0, \dots, q+1 \ . \tag{31}$$

For $j = 0$ the statement is trivial. For $j > 0$,

$$\langle x^j|u_i\rangle = \langle \chi x^{j-1}|u_i\rangle = \langle x^{j-1}|\chi u_i\rangle = \Lambda_i \langle x^{j-1}|u_i\rangle \ . \tag{32}$$

This provides the recursive step proving (31), the full result follows by linearity. □

χ is an approximation of the operator x and this lemma shows that $\{u_i\}$, the eigenfunctions of χ, share with δ functions, which are "eigenfunctions" of x, the property that projection of a function on either is done by its evaluation at the appropriate eigenvalue. This similarity is the reason for the name we give to the δ lemma.

With this lemma it is almost immediate to prove the main result of this subsection:

Theorem 7 *Let f be a polynomial of degree at most $2q+1$. Then*

$$\int_\Omega w(x)f(x)dx = \sum_{i=0}^{q} \langle 1|u_i\rangle^2 f(\Lambda_i) \ , \tag{33}$$

i.e. the quadrature rule

$$\int_\Omega w(x)f(x)dx \approx \sum_{i=0}^{q} \langle 1|u_i\rangle^2 f(\Lambda_i) \tag{34}$$

is exact of degree $2q+1$.

Proof Again we prove the result for $f(x) = x^j$, $j = 0, \ldots, 2q+1$, the full result follows by linearity. For $j \geq 1$, choose integers n_1, n_2 between 0 and q such that $j = n_1 + n_2 + 1$. We then have

$$\begin{aligned}\int_\Omega w(x)x^j dx &= X(x^{n_1}, x^{n_2}) = X\left(\sum_{k=0}^{q}\langle x^{n_1}|u_k\rangle u_k, \sum_{i=0}^{q}\langle x^{n_2}|u_i\rangle u_i\right) \\ &= \sum_{i=0}^{q}\langle 1|u_i\rangle^2 \Lambda_i^j \ .\end{aligned} \tag{35}$$

In the last step we have used the δ lemma twice.

For $j = 0$ observe that

$$\int_\Omega w(x)dx = \langle 1|1\rangle = \left\langle \sum_{k=0}^{q}\langle 1|u_k\rangle u_k \,\middle|\, \sum_{i=0}^{q}\langle 1|u_i\rangle u_i \right\rangle = \sum_{i=0}^{q}\langle 1|u_i\rangle^2 \ , \tag{36}$$

by the orthonormality of the u_i. □

Theorem 7 relates the spectrum of χ to the nodes of Gaussian quadrature. It is in fact easy to prove other facts in the theory of Gaussian quadrature using our approach. For example, to see that none of the weights vanish just take $p = u_i$ in the δ lemma. To see that when Ω is a single interval $[a, b]$ the nodes must be in its interior just observe that

$$\begin{aligned} b - \Lambda_i &= \int_a^b w(x)(b-x)u_i(x)^2\, dx > 0, \\ a - \Lambda_i &= \int_a^b w(x)(a-x)u_i(x)^2\, dx < 0 \ .\end{aligned} \tag{37}$$

We also obtain the following widely known characterization of the nodes:

Theorem 8 *The nodes Λ_i are roots of any nontrivial degree $q+1$ polynomial orthogonal to $\mathcal{P}_q$.*

Proof Let p be a nontrivial degree $q+1$ polynomial orthogonal to $\mathcal{P}_q$. Then using the δ lemma, $0 = \langle p|u_i\rangle = \langle 1|u_i\rangle p(\Lambda_i)$. Since $\langle 1|u_i\rangle$ is nonzero, this gives $p(\Lambda_i) = 0$. □

Our presentation on Gaussian quadrature is the reverse of that in [7], [11]. The starting point in [7], [11] is that the nodes in degree $2q+1$ Gaussian quadrature are roots of the degree $q+1$ polynomial p from theorem 8; it is then shown that the eigenvalues of a matrix representation of χ are equal to these. Here we have gone in the other direction; without *a priori* assumption of the existence of a Gaussian quadrature formula, we have shown that the eigenvalues of χ are quadrature nodes and as a consequence of the δ lemma we also obtain the fact that they are roots of the degree $q+1$ polynomial p from theorem 8.

As we shall see in the next subsection, our approach to Gaussian quadrature allows a generalization to higher dimensions. However, in the generalization of the δ lemma the polynomial p is restricted to $\mathcal{P}_q$, not $\mathcal{P}_{q+1}$. This means that theorem 8 cannot be easily generalized to multi dimensions. The characterization of cubature nodes as roots of polynomials requires elaborate analysis, see [20], [22]. However the characterization of nodes as eigenvalues is naturally obtained from our approach, as we now set out to show.

4.2 Generalization to Cubature

We denote by $\mathcal{P}_q$ the $n = \binom{d+q}{d}$ dimensional vector space of polynomials in d variables $x_1, \ldots, x_d$ of total degree up to q (total degree is defined by degree$(x_1^{m_1} x_2^{m_2} \ldots x_d^{m_d}) = m_1 + m_2 + \ldots + m_d$).

An N-point d-dimensional cubature formula

$$\int_\Omega w(x) f(x) d^d x \approx \sum_{\alpha=1}^{N} w_\alpha f(x_\alpha) \tag{38}$$

is said to be of degree D if it is exact whenever $f(x)$ is a polynomial of total degree at most D and non-exact for at least one polynomial of total degree $D+1$. Here Ω is a suitable region in $\mathbf{R}^d$ and $w(x) \geq 0$ a suitable weight function. The weights w_α are assumed positive.

We supply $\mathcal{P}_q$ with the inner product

$$\langle a|b\rangle = \int_\Omega w(x) a(x) b(x)\, d^d x\ , \qquad \forall\, a,\ b \in \mathcal{P}_q\ , \tag{39}$$

and define Π_q, the orthogonal projection operator from $\mathcal{P}_{q+1}$ onto $\mathcal{P}_q$ with respect to the above inner product, in the obvious way. We can then define d self adjoint operators $\chi_1, \ldots, \chi_d$ on $\mathcal{P}_q$ by

$$\chi_i p = \Pi_q x_i p\ , \qquad \forall p \in \mathcal{P}_q\ , \tag{40}$$

with related symmetric bilinear forms $X_i : \mathcal{P}_q \times \mathcal{P}_q \to \mathbf{R}$,

$$X_i(a, b) = \langle a|\chi_i b\rangle = \int_\Omega w(x)a(x)x_i b(x)\, d^d x \qquad \forall a, b \in \mathcal{P}_q\ . \tag{41}$$

Generally $[\chi_i,\ \chi_j] \neq 0$ so we can not find a basis of $\mathcal{P}_q$ in which all the χ_i are simultaneously diagonalised, and we do not have a direct analog of the one-dimensional case in which the eigenvalues of the single operator χ served as quadrature nodes. We shall show, however, that there is a correspondence between cubature rules and spectra of certain commuting extensions of matrix representations of the operators $\chi_1, \ldots,\ \chi_d$. As a first step towards this we prove the following:

Theorem 9 *Let the $n \times n$ matrices $A_1, \ldots, A_d$ be the representations of the operators $\chi_1, \ldots, \chi_d$ in an arbitrary orthonormal basis $\{e_a\}$ of $\mathcal{P}_q$ (so $(A_i)_{ab} = \langle e_a|\chi_i e_b\rangle$). Suppose that for the region Ω and weight function $w(x)$ we have a degree $2q+1$, N point cubature rule with positive weights. Then there exist $N \times N$ symmetric commuting extensions of $A_1, \ldots, A_d$.*

Proof Suppose the cubature rule takes the form

$$\int_\Omega w(x) f(x) d^d x \approx \sum_{\alpha=1}^{N} w_\alpha f(x_\alpha)\ . \tag{42}$$

Then, since all integrands are of degree at most $2q + 1$, we have

$$\delta_{ab} = \langle e_a|e_b\rangle = \int_\Omega w(x)e_a(x)e_b(x)d^d x = \sum_{\alpha=1}^{N} w_\alpha e_a(x_\alpha)e_b(x_\alpha)\ , \tag{43}$$

$$\begin{aligned}(A_i)_{ab} = \langle e_a|\chi_i e_b\rangle &= \int_\Omega w(x)e_a(x)x_i e_b(x)d^d x \\ &= \sum_{\alpha=1}^{N} w_\alpha e_a(x_\alpha)(x_\alpha)_i e_b(x_\alpha)\ .\end{aligned} \tag{44}$$

Define the $n \times N$ matrix Q by

$$Q_{a\alpha} = \sqrt{w_\alpha} e_a(x_\alpha)\ , \tag{45}$$

and $N \times N$ diagonal matrices $\Lambda_1\ \ldots, \Lambda_d$ with diagonal entries $(\Lambda_i)_{\alpha\alpha} = \Lambda_{i\alpha}$,

$$\Lambda_{i\alpha} = (x_\alpha)_i\ . \tag{46}$$

Equations (43)–(44) read

$$I_{n\times n} = QQ^T\ , \qquad A_i = Q\Lambda_i Q^T\ . \tag{47}$$

Using theorem 5 in section 2 we conclude that $A_1, \ldots, A_d$ have $N \times N$ symmetric commuting extensions. □

It is natural to ask whether the matrix commuting extensions of theorem 9 are representations of commuting extensions of the operators $\{\chi_i\}$ in some N dimensional space of functions V which includes $\mathcal{P}_q$ as a subspace. In other words, is it possible to extend the basis $\{e_a\}$ of $\mathcal{P}_q$ to an orthonormal basis of V by adding $N-n$ orthonormal functions $e_{n+1}, \ldots, e_N$ in such a way that the $N \times N$ matrices $(\tilde{A}_i)_{\alpha,\beta} = \langle e_\alpha | x_i e_\beta \rangle = \int_\Omega w(x) e_\alpha(x) x_i e_\beta(x)\, d^d x$ commute? Unfortunately, in all but the simplest cases, we could not find, nor prove the existence of, such functions $e_{n+1}, \ldots, e_N$. The answer may be possibly based on Xu's construction of interpolating multi dimensional polynomials [20], [21]. However, even though we can not view the matrix commuting extensions of theorem 9 as representations of operator extensions of the χ_i, they do satisfy a certain compatibility condition with the χ_i which we prove in theorem 10.

Let us introduce the N dimensional vector space $V(=\mathbf{R}^N)$, with the standard inner product, whose elements we denote in bold face. $\mathcal{P}_q$ is mapped to a subspace of V by the inclusion operator $\iota : \mathcal{P}_q \to V$ which is defined by $\iota e_1 = \mathbf{e_1}, \ldots, \iota e_n = \mathbf{e_n}$, where $\{\mathbf{e_a}\}$ are the first n members of the standard basis of V. Extend $\{\mathbf{e_a}\}$ to an orthonormal basis $\{\mathbf{e}_\alpha\}$ of V by adding any orthonormal basis $\{\mathbf{e_{n+1}}, \ldots, \mathbf{e_N}\}$ of the orthogonal complement of $\mathrm{span}(\{\mathbf{e_a}\})$ in V. Even though our attempts to extend $\mathcal{P}_q$ with functions failed, now we are extending with N-tuples. Define the obvious projection operator $\pi : V \to \mathcal{P}_q$ by $\pi \mathbf{e_1} = e_1, \ldots, \pi \mathbf{e_n} = e_n$, $\pi \mathbf{e_{n+1}} = \ldots = \pi \mathbf{e_N} = 0 \in \mathcal{P}_q$; clearly $\pi\iota = I$, the identity operator on $\mathcal{P}_q$.

Recall that the essential step in the proof of theorem 5 is extension of Q to an $N \times N$ orthonormal matrix $\tilde{Q}$ by appending any $N-n$ orthonormal rows. In this way $\tilde{A}_1, \ldots, \tilde{A}_d$, $N \times N$ symmetric commuting extensions of the A_i are constructed in theorem 9, where $\tilde{A}_i = \tilde{Q}\Lambda_i\tilde{Q}^T$. Since the $\tilde{A}_1, \ldots, \tilde{A}_d$ mutually commute and are symmetric, there exist N orthonormal common eigenvectors $\mathbf{u}_\alpha \in V$, such that $\tilde{A}_i \mathbf{u}_\alpha = \Lambda_{i\alpha}\mathbf{u}_\alpha$. The matrices $\tilde{A}_i$ are given in the basis $\{\mathbf{e}_\alpha\}$ and $\tilde{Q}$ is the transformation between this basis and the eigenvector basis $\{\mathbf{u}_\alpha\}$. Note that the rows of $\tilde{Q}$ give the coordinates of the vectors $\{\mathbf{e}_\alpha\}$ in the basis $\{\mathbf{u}_\alpha\}$, hence the extension of Q to $\tilde{Q}$ by adding arbitrary $N-n$ orthonormal rows is nothing but the extension of $\{\mathbf{e_a}\}$ to $\{\mathbf{e}_\alpha\}$ the orthonormal basis of V described above. The reader is reminded that at present we are assuming the existence of a cubature formula hence the eigenvalues $\Lambda_{i\alpha}$ are defined in (46). We can now state:

Theorem 10 *The commuting extensions of theorem 9, $\{\tilde{A}_i\}$, satisfy the following compatibility condition with the operators $\{\chi_i\}$,*

$$\tilde{A}_i \iota p = \iota x_i p = \iota \chi_i p, \qquad \forall p \in \mathcal{P}_{q-1}\ , \tag{48}$$

where $\mathcal{P}_{q-1}$ is regarded in the natural way as a subspace of $\mathcal{P}_q$.

Note Applying π to (48) gives $\pi\tilde{A}_i\iota p = \chi_i p$, for $p \in \mathcal{P}_{q-1}$, which is automatic as $\tilde{A}_i$ is an extension of A_i. However, (48) contains more information than this, and is not true for an arbitrary extension of A_i.

Proof We first prove that for any $p \in \mathcal{P}_q$ and any eigenvector $\mathbf{u}_\alpha$,

$$\langle \iota p | \mathbf{u}_\alpha \rangle = \sqrt{w_\alpha}\, p(x_\alpha)\ , \tag{49}$$

where w_α, x_α, are the weights and nodes of the cubature formula whose existence is assumed in theorem 9. We already noted that the rows of $\tilde{Q}$ from the proof of theorem 9 give the coordinates of the N vectors $\mathbf{e}_\alpha$ in the basis $\{\mathbf{u}_\alpha\}$, in particular the rows of Q give the coordinates of $\mathbf{e_a} = \iota e_a$, $a = 1, \dots, n$. Recall that $Q_{a\alpha} = \sqrt{w_\alpha} e_a(x_\alpha)$, thus (49) is proven for basis elements $e_a \in \mathcal{P}_q$. The proof for general $p \in \mathcal{P}_q$ follows by linearity.

We now expand the left hand side of (48) in the basis $\{\mathbf{u}_\alpha\}$. For any $p \in \mathcal{P}_{q-1}$

$$\langle \tilde{A}_i \iota p | \mathbf{u}_\alpha \rangle = \Lambda_{i\alpha} \langle \iota p | \mathbf{u}_\alpha \rangle = \Lambda_{i\alpha} \sqrt{w_\alpha} p(x_\alpha) = \sqrt{w_\alpha} (x_\alpha)_i p(x_\alpha) \ , \tag{50}$$

using (49) and (46) respectively in the last two steps. To expand the right hand side of (48) note that $x_i p = \chi_i p \in \mathcal{P}_q$ for all $p \in \mathcal{P}_{q-1}$. Invoking (49) again we obtain

$$\langle \iota x_i p | \mathbf{u}_\alpha \rangle = \sqrt{w_\alpha} (x_\alpha)_i p(x_\alpha) \ , \tag{51}$$

which completes the proof. □

Note that taking $p = 1$ in (49) gives $w_\alpha = \langle \iota 1 | \mathbf{u}_\alpha \rangle^2$. In theorem 9 we saw that the eigenvalues of the commuting extensions are related to cubature nodes, here we obtain a relation between the weights and common eigenvectors.

We shall see in section 4.3 that with an appropriate choice of basis the compatibility condition of theorem 10 implies that the commuting extensions have certain off-diagonal zero blocks; in particular this special structure aids computation of commuting extensions.

The obvious question to ask at this stage is whether there is a converse of theorems 9 and 10. That is, suppose we have $\tilde{A}_1, \dots, \tilde{A}_d$, $N \times N$ symmetric commuting extensions of $A_1, \dots, A_d$, which satisfy the compatibility condition $\tilde{A}_i \iota p = \iota \chi_i p = \iota x_i p$, $\forall p \in \mathcal{P}_{q-1}$. Can we build a cubature rule, without *a priori* assumption of its existence, using the eigenvalues and eigenvectors of $\tilde{A}_1, \dots, \tilde{A}_d$? In theorem 11 we give an affirmative answer to this. The treatment follows the presentation on Gaussian quadrature from section 4.1; in particular we start with a δ lemma. Note that given the commuting matrices $\tilde{A}_i$ we can find their diagonal representations Λ_i, but we do not assume in advance any connection of the Λ_i with cubature nodes.

Lemma 2 *(The multidimensional δ lemma) Suppose the commuting extensions satisfy the compatibility condition $\tilde{A}_i \iota \grave{p} = \iota x_i \grave{p} = \iota \chi_i \grave{p}$ for all $i = 1, \dots, d$, and for all $\grave{p} \in \mathcal{P}_{q-1}$. Then, for any $p \in \mathcal{P}_q$*

$$\langle \iota p | \mathbf{u}_\alpha \rangle = \langle \iota 1 | \mathbf{u}_\alpha \rangle \ p(\lambda_\alpha) \ , \tag{52}$$

where the points $\lambda_\alpha \in \mathbf{R}^d$ have entries $(\Lambda_{1\alpha}, \dots, \Lambda_{d\alpha})$, all eigenvalues of $\tilde{A}_1$, $\dots$, $\tilde{A}_d$, satisfying $A_i \mathbf{u}_\alpha = \Lambda_{i\alpha} \mathbf{u}_\alpha$.

Proof We prove (52) for monomials $p = x_1^{m_1} x_2^{m_2} \dots x_d^{m_d}$. For $p = 1$ the statement is trivial. For any other monomial $p \in \mathcal{P}_q$ we can write $p = x_i \grave{p}$, where $\grave{p} \in \mathcal{P}_{q-1}$. Then

$$\langle \iota p | \mathbf{u}_\alpha \rangle = \langle \iota x_i \grave{p} | \mathbf{u}_\alpha \rangle = \langle \tilde{A}_i \iota \grave{p} | \mathbf{u}_\alpha \rangle = \langle \iota \grave{p} | \tilde{A}_i \mathbf{u}_\alpha \rangle = \Lambda_{i\alpha} \ \langle \iota \grave{p} | \mathbf{u}_\alpha \rangle \ . \tag{53}$$

Here the compatibility condition was used in the second step. Repeated application of (53) completes the proof for monomial p; the full result follows by linearity. □

Note Recall that we do not know how to relate V to a space of polynomials (or other functions) in a way which gives commuting extensions of the operators $\chi_1, \ldots, \chi_d$. In particular, we can not interpret the eigenvectors $\mathbf{u}_\alpha$ as polynomials (or other functions). Thus our present state of understanding allows us to view the $\mathbf{u}_\alpha$ as "δ *vectors*" in V and not as δ *functions*, which was possible in the 1-dimensional case. Moreover we can not identify $\mathcal{P}_{q+1}$ with a subspace of V. Hence, in contrast to the one dimensional case, we restrict $p \in \mathcal{P}_q$ in the multidimensional δ lemma thereby losing the immediate connection between cubature nodes and roots of polynomials in $\mathcal{P}_q^\perp$. Again, Xu's work [20], [21] may provide a key to this problem.

We are now fully prepared for the converse statement to theorems 9 and 10:

Theorem 11 *Let $A_1, \ldots, A_d$ be the representation of the operators $\chi_1, \ldots, \chi_d$ in an orthonormal basis $\{e_a\}$ of $\mathcal{P}_q$. Let $\tilde{A}_1, \ldots, \tilde{A}_d$ be $N \times N$ symmetric commuting extensions of $A_1, \ldots, A_d$ satisfying the compatibility condition $\tilde{A}_i \iota p = \iota x_i p = \iota \chi_i p$ for all $p \in \mathcal{P}_{q-1}$. Then for every polynomial f in $\mathcal{P}_{2q+1}$*

$$\int_\Omega w(x) f(x) d^d x = \sum_{\alpha=1}^{N} \langle \iota 1 | \mathbf{u}_\alpha \rangle^2 f(\lambda_\alpha) \,. \tag{54}$$

Here the $\mathbf{u}_\alpha$ are joint eigenvectors of $\tilde{A}_1, \ldots, \tilde{A}_d$, satisfying $A_i \mathbf{u}_\alpha = \Lambda_{i\alpha} \mathbf{u}_\alpha$, and the points $\lambda_\alpha \in \mathbf{R}^d$ have entries $(\Lambda_{1\alpha}, \ldots, \Lambda_{d\alpha})$.

Proof Recall the symmetric bilinear forms X_i on $\mathcal{P}_q$ defined in (41). Given the commuting extensions, we can introduce symmetric bilinear forms $\tilde{X}_i$ on V defined by $\tilde{X}_i(\mathbf{u}, \mathbf{v}) = \langle \mathbf{u} | \tilde{A}_i \mathbf{v} \rangle$. Since the $\tilde{A}_i$ are extensions of the A_i we have $X(p_1, p_2) = \tilde{X}_i(\iota p_1, \iota p_2)$ for all p_1, p_2 in $\mathcal{P}_q$. The $\tilde{X}_i$ are simultaneously diagonalized in the basis $\{\mathbf{u}_\alpha\}$, $\tilde{X}_i(\mathbf{u}_\alpha, \mathbf{u}_\beta) = \Lambda_{i\alpha} \delta_{\alpha\beta}$.

It is sufficient to prove the statement of the theorem for monomials. For $f = 1$ we have

$$\int_\Omega w(x) d^d x = \langle 1 | 1 \rangle = \langle \iota 1 | \iota 1 \rangle = \left\langle \sum_{\alpha=1}^{N} \langle \iota 1 | \mathbf{u}_\alpha \rangle \mathbf{u}_\alpha \,\middle|\, \sum_{\beta=1}^{N} \langle \iota 1 | \mathbf{u}_\beta \rangle \mathbf{u}_\beta \right\rangle = \sum_{\alpha=1}^{N} \langle \iota 1 | \mathbf{u}_\alpha \rangle^2, \tag{55}$$

by the orthonormality of the $\mathbf{u}_\alpha$. Note that in the second expression in (55) the inner product is taken in $\mathcal{P}_q$, in subsequent expressions it is taken in V.

Any other monomial in $\mathcal{P}_{2q+1}$ can be written in the form $f = x_i f_1 f_2$ for some monomials $f_1, f_2 \in \mathcal{P}_q$ and some i. Note that use of the multidimensional δ lemma is possible since we assume the $\tilde{A}_i$ satisfy the compatibility condition, and so

$$\begin{aligned}\int_\Omega w(x) f(x) d^d x &= \int_\Omega w(x) f_1(x) x_i f_2(x) \; d^d x = X_i(f_1, f_2) \\ &= \tilde{X}_i(\iota f_1, \iota f_2) = \tilde{X}_i \left(\sum_{\alpha=1}^{N} \langle \iota f_1 | \mathbf{u}_\alpha \rangle \mathbf{u}_\alpha, \sum_{\beta=1}^{N} \langle \iota f_2 | \mathbf{u}_\beta \rangle \mathbf{u}_\beta \right)\end{aligned}$$

$$= \sum_{\alpha=1}^{N} \Lambda_{i\alpha} \langle \iota f_1 | \mathbf{u}_\alpha \rangle \langle \iota f_2 | \mathbf{u}_\alpha \rangle = \sum_{\alpha=1}^{N} \langle \iota 1 | \mathbf{u}_\alpha \rangle^2 \Lambda_{i\alpha} f_1(\lambda_\alpha) f_2(\lambda_\alpha)$$
$$= \sum_{\alpha=1}^{N} \langle \iota 1 | \mathbf{u}_\alpha \rangle^2 f(\lambda_\alpha) \; . \tag{56}$$

Thus (54) is proven for monomial f; the full result follows by linearity. □

Theorems 9,10,11 give the main result of this paper, that N point, odd order cubature formulae with positive weights are equivalent to symmetric commuting extensions, satisfying the compatibility condition, of matrix representations of the operators $\chi_1, \dots, \chi_d$.

4.3 Discussion and Consequences

Our findings suggest a computational approach to the derivation of cubature formulae. If appropriate commuting extensions are numerically found their simultaneous diagonalisation will give the cubature rule in (54). To numerically obtain the matrices $\{A_i\}$ we introduce an orthonormal basis of $\mathcal{P}_q$ consisting of an orthonormal basis of $\mathcal{P}_0$ (a constant function e_1 with $\|e_1\| = \sqrt{\langle e_1 | e_1 \rangle} = 1$), extended to one of $\mathcal{P}_1$, extended to one of $\mathcal{P}_2$ etc., *i.e.* a basis $\{e_a\}$, $a = 1, \dots, n = \binom{d+q}{d}$, such that

$$\begin{aligned} &e_1 \text{ is an orthonormal basis of } \mathcal{P}_0 \\ &e_1, \dots, e_{d+1} \text{ is an orthonormal basis of } \mathcal{P}_1 \\ &e_1, \dots, e_{\frac{1}{2}(d+1)(d+2)} \text{ is an orthonormal basis of } \mathcal{P}_2 \\ &\text{etc.} \end{aligned} \tag{57}$$

Such a basis can be obtained from the monomials $\{x_1^{m_1} \dots x_d^{m_d}\}$, $m_1 + \dots + m_d \le q$, by the Gram-Schmidt procedure. Note that all basis elements e_a of degree m or more are orthogonal to $\mathcal{P}_{m-1}$. This choice of basis and the fact that $\{A_i\}$ represent the operators $\{\chi_i\}$ imply that the A_i have tridiagonal block form as in (19), with $q+1$ blocks on the diagonal. In the notation of section 3, $n_1 = 1$ and for $m = 2, 3, \dots, q+1$, $n_m = \dim\mathcal{P}_{m-1} - \dim\mathcal{P}_{m-2}$ ($n_1 = 1$, $n_2 = d$, $n_3 = d(d+1)/2$ etc). Moreover, the commutator of any pair of A_i's is zero apart from a single block of size $\binom{q+d-1}{d-1} \times \binom{q+d-1}{d-1}$ in the bottom right hand corner (note $\binom{q+d-1}{d-1} = n_{q+1} = \dim\mathcal{P}_q - \dim\mathcal{P}_{q-1}$). The compatibility condition, together with the fact that $\mathbf{e_{n+1}}, \dots, \mathbf{e_N}$ are orthogonal to $\iota\mathcal{P}_q$, imply that the bottom left $(N-n) \times \dim(\mathcal{P}_{q-1})$ block of $\tilde{A}_i$ is zero and by symmetry so is the corresponding block in the upper right. Thus the commuting extensions $\{\tilde{A}_i\}$ we seek are precisely those in tridiagonal block form as in section 3, and finding them is equivalent to solving the system of equations (21). Note also that since our first basis element e_1 is a constant polynomial the cubature weights are obtained from the first entries of the eigenvectors $\mathbf{u}_\alpha$, $w_\alpha = \langle \iota 1 | \mathbf{u}_\alpha \rangle^2 = \frac{1}{e_1^2} \langle \iota e_1 | \mathbf{u}_\alpha \rangle^2 = \left(\frac{(\mathbf{u}_\alpha)_1}{e_1} \right)^2$.

In the case $d = 2$, we note that the matrices A_1, A_2 have $n_{r-1} = q$ and $n_r = q + 1$ in the notation of section 3, and thus from (26), which is based on counting degrees of freedom, the expected size of the commuting extensions is

$$N \geq n + \frac{q(q+1)}{6} \; . \tag{58}$$

Using $n = \dim\mathcal{P}_q = \frac{1}{2}(q+1)(q+2)$ we obtain

$$N \geq \frac{(2q+2)(2q+3)}{6} = \frac{1}{3}\dim\mathcal{P}_{2q+1} \; . \tag{59}$$

This is exactly the number of nodes we expect from counting degrees of freedom in a 2-dimensional cubature formula of degree $2q + 1$.

For $d > 2$ the A_i have a more subtle structure that requires refinement of the discussion leading to equation (26). However, the equivalence of cubature formulae and commuting extensions (satisfying the compatibility condition) allows us to estimate N by easily counting degrees of freedom in a general d-dimensional cubature formula of degree $2q + 1$. Thus,

$$N \geq \frac{1}{d+1}\dim\mathcal{P}_{2q+1} \; . \tag{60}$$

We emphasize again that such calculations are not rigorous and the inequalities obtained in this way can serve only as recomendations for the choice of N, indeed certain cubature formulas with fewer points are known.

Before going on we present two theoretical consequences of the equivalence between cubature formulae and commuting extensions.

Theorem 12 *Let N be the number of nodes in a degree $2q + 1$, d-dimensional positive weight cubature rule. Then*

$$N \geq \binom{d+q}{d} + \frac{1}{2}\max_{i,j}\mathrm{rank}([A_i, A_j]) \; , \tag{61}$$

where $A_1, \dots, A_d$ are the matrix representations of the operators $\chi_1, \dots, \chi_d$ on $\mathcal{P}_q$.

Proof By theorem 9 an N point cubature rule gives $N \times N$ commuting extensions of the matrices A_i. By theorem 2, section 2, the size of such extensions is at least $\dim\mathcal{P}_q + \frac{1}{2}\max_{i,j}\mathrm{rank}([A_i, A_j])$. □

Notes (1) As mentioned in the introduction, theorem 12 has its origins in the work of Möller [13]. A statement of the result in a form that clearly corresponds to our statement can be found in [4], which cites [14] and [19]. Our proof, however, is a substantial simplification.

(2) It is informative to compare the lower bound of theorem 12 with estimates based on parameter counting. As a consequence of our previous remarks on the block structure of $[A_i, A_j]$

$$\mathrm{rank}([A_i, A_j]) \leq \binom{d-1+q}{d-1} = \frac{d}{d+q}\binom{d+q}{d} \; , \tag{62}$$

so the second term in (61) is typically a small fraction of the first term. Consequently for large q the right hand side of (61) is much smaller than the number of nodes we expect from counting degrees of freedom in a degree $2q+1$, d-dimensional cubature formula, which is

$$\left\lceil \frac{1}{d+1}\binom{d+2q+1}{d} \right\rceil. \tag{63}$$

This comparison indicates why the lower bound on the number of points needed for a cubature formula is rarely attained.

Theorem 13 *Let $A_1, \dots, A_d$ be matrix representations of $\chi_1, \dots, \chi_d$. In any degree $2q+1$, d-dimensional, positive weight cubature rule, and for each i, there is a node x_α with $(x_\alpha)_i$ less than or equal to the smallest eigenvalue of A_i, and a node x_β with $(x_\beta)_i$ greater than or equal to the largest eigenvalue of A_i.*

Proof By theorem 9 a cubature rule of degree $2q+1$ gives commuting extensions of the matrices A_i with the nodes composed of the eigenvalues of the extended matrices. By theorem 6 in section 2 the smallest/largest eigenvalue of the extended matrices is less/greater than or equal to the smallest/largest eigenvalue of the matrices before extension. □

Note As far as we are aware this theorem is not even known for $d=1$. For $d=1$ the theorem says that any N-point, positive weight, degree $2q+1$ quadrature rule must have a node less/greater than or equal to the smallest/largest Gaussian quadrature node. Thus Gaussian quadrature has the property that the span of the nodes is the smallest possible, amongst all positive weight quadrature rules, with any number of points, that are exact to the same degree.

Xu has earlier recognized the possibility of calculating cubature formulae via solving a system of equations similiar to (21), equations (7.1.6)–(7.1.9) in [20]. However equations (21) may be easier to use, partly because they are quadratic whereas Xu's equations are quartic.

Our efforts to construct cubature formulae via commuting extensions yielded an algorithm for calculating general Radon type formulae (*i.e.*7 node, degree 5, cubature rules for two variable integrals with general Ω, $w(x_1, x_2)$). Several Radon formulas for non standard domains were found. In [9], we describe the calculation via commuting extensions of several new formulae of degrees 13, 15, 17 for $\Omega = \mathbf{R}^2$, $w(x_1, x_2) = \exp(-x_1^2 - x_2^2)$. It seems that our degree 17 formula has the least number of nodes of all known formulae (as listed in [5]).

In all our calculations the simultaneous diagonalization was easily done using the algorithm from [1].

5 Summary and open questions

The central results of this paper are theorems 9,10,11, which prove the equivalence of cubature formulae and commuting extensions satisfying the compatibility condition (equivalent in an appropriate basis to requiring certain zero blocks in the extension matrices). This raises the questions of existence and methods of computation for commuting extensions. Our knowledge of the theory of commuting extensions is summarized by theorems 1 to 6, and in the end of section 2 we have briefly described our initial attempts at their computation.

There is clearly enormous potential for further work here. In the context of our main topic, the connection between cubature formulae and commuting extensions, there is one open issue mentioned several times in section 5: We have not yet presented an interpretation of the vector space V, on which the commuting extensions act, as a space of functions (or maybe even polynomials). For numerical work in quantum mechanics it would be a major advantage if we could construct finite dimensional function spaces containing the space of all polynomials of a given degree as a subspace, on which the natural projections of the operators x_i commute. The existence (or nonexistence) of such spaces is a topic we hope to investigate. Possible connections with Xu's work [20], [21] were indicated, see also [2].

Another question left open in our work is that we have not given an existence proof of cubature formulae from the commuting extension viewpoint. Although theorem 1 in section 2 guarantees the existence of commuting extensions of an arbitrary set of matrices, it does not guarantee extensions in the form required for application of theorem 11. An existence proof for commuting extensions of this form would provide an alternative approach to *Tchakaloff's theorem* [17] that guarantees (for any suitable domain Ω and weight function $w(x)$) the existence of positive weight cubature rules that are exact for certain sets of functions.

The numerical question of computing cubature formulae is now subsumed under the more general question of computing commuting extensions; likewise the open sore that there is no good way to predict the minimal number of points needed for a cubature rule is now subsumed under the question of finding the minimal dimension for commuting extensions. There are a number of points in the theory of commuting extensions which we feel may be improved, for example, existence of symmetric commuting extensions for symmetric matrices may well be provable, but we suspect the question of minimal dimension is extremely difficult. Fortunately, just because it is difficult theoretically does not mean answers cannot be found numerically, and we are hopeful that good algorithms can be devised that find commuting extensions of a given dimension, if they exist. The determining equations are linear and quadratic, and although there surely will be ill-conditioning in certain cases, it is hard to see why this should be so in general. Our attempts to compute commuting extensions numerically are at an initial and tentative stage; there is much more that can be tried here.

Another aspect to be considered in construction of cubature formulae/commuting extensions is symmetry in the domain Ω and weight $w(x)$. This will clearly influence the matrices A_i, which represent the natural projections of the operators x_i, and should be respected in construction of the extensions $\tilde{A}_i$, see also [2].

We hope very much that more applications will emerge for the notion of commuting extensions. The idea that noncommutativity can be resolved by introducing extra dimensions is a very natural one. In fact, we suspect that, more than the ranks or the norms of commutators, the size of minimal commuting extensions is probably the best measure of how noncommuting a set of matrices is.

The minimal size issue appears in other settings too. For example, given a set of $m \times n$ matrices A_i we can ask what is the smallest N such that there exist an $m \times N$ matrix U and an $n \times N$ matrix V, both with orthonormal rows, and $N \times N$

diagonal matrices Λ_i, such that $A_i = U\Lambda_i V^T$. In our context, this provides a natural generalization of the singular value decomposition of a single matrix, in the same way that (26) provides the generalization of diagonalization of a single symmetric matrix.

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