A moment matrix approach to computing symmetric cubatures

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Cubature: quadrature in higher dimension

$\mathcal{D} \subset \mathbb{R}^n$ compact $\qquad \mathbb{R}[x] = \mathbb{R}[x_1, \dots, x_n]$

$$\Omega : \begin{array}{rcl} \mathbb{R}[x] & \to & \mathbb{R} \\ f & \mapsto & \int_{\mathcal{D}} f(x)\,dx \end{array}$$

A *cubature of degree* d for Ω is a linear form

$$\Lambda : \begin{array}{rcl} \mathbb{R}[x] & \to & \mathbb{R} \\ f & \mapsto & \sum_{j=1}^{r} a_j f(\xi_j) \end{array}$$

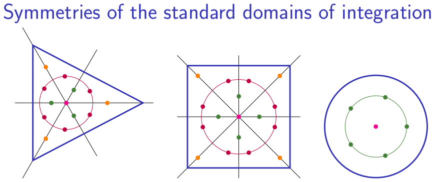
with $a_j > 0$ and $\xi_j \in \mathcal{D}$

such that $\quad \Omega(f) = \Lambda(f), \quad \forall f \in \mathbb{R}[x]_{\leq d}$.

The coefficients a_j are the *weights*. The points ξ_j are the *nodes*.

$$r \geq \dim \mathbb{R}[x]_{\leq \lfloor \frac{d}{2} \rfloor}$$

Symmetries of the standard domains of integration



D_3 $\qquad D_4$ $\qquad C_5$

Gaussian quadrature of degree d=2 r-1

Moments: $\mu_k = \int_{-1}^{1} x^k\,\omega(x)\,dx, \quad k = 0, \dots, 2r-1$

Equations for the nodes and weights:

$$\mu_k = \sum_{j=1}^{r} a_j \xi_j{}^k, \quad k = 0, \dots, 2r-1$$

If you know the nodes, you get the weights as:

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \xi_1 & \xi_2 & \cdots & \xi_r \\ \vdots & \vdots & & \vdots \\ \xi_1{}^{r-1} & \xi_2{}^{r-1} & \cdots & \xi_r{}^{r-1} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_r \end{pmatrix} = \begin{pmatrix} \mu_0 \\ \mu_1 \\ \vdots \\ \mu_{r-1} \end{pmatrix}.$$

To determine the nodes: $(\mu_k)_k$ is a solution to the recurrence equation

$$\mu_{k+r} = \pi_{r-1}\mu_{k+r-1} + \dots + \pi_0 \mu_k$$

Thus:

$$\underbrace{\begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{r-1} \\ \mu_1 & & \iddots & \vdots \\ \vdots & \iddots & & \\ \mu_{r-1} & & \cdots & \mu_{2r-2} \end{pmatrix}}_{H_1} \underbrace{\begin{pmatrix} & & & \pi_0 \\ 1 & & & \pi_1 \\ & \ddots & & \vdots \\ & & 1 & \pi_{r-1} \end{pmatrix}}_{M_x} = \underbrace{\begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_r \\ \mu_2 & & \iddots & \vdots \\ \vdots & \iddots & & \\ \mu_r & & \cdots & \mu_{2r-1} \end{pmatrix}}_{H_x}.$$

The eigenvalues of $M_x = H_1^{-1} H_x$ are the roots of

$$\pi(\xi) = \xi^r - \pi_{r-1}\xi^{r-1} - \dots - \pi_1 \xi - \pi_0 = \prod_{j=1}^{r} (\xi - \xi_j).$$

Symmetry and block diagonalisation for quadrature

$$\Omega(f) = \int_{-1}^{1} f(x)dx = \int_{0}^{1} (f(x) + f(-x))dx \qquad \mu_k = \int_{-1}^{1} x^k dx$$

The matrix H_1 of the scalar product $(p, q) = \int_{-1}^{1} p(x)q(x)dx$ is

$$\begin{pmatrix} \mu_0 & 0 & \mu_2 & 0 & \dots & \mu_{r-1} \\ 0 & \mu_2 & 0 & & \iddots & \vdots \\ \mu_2 & 0 & & \iddots & & \vdots \\ 0 & & \iddots & & & \vdots \\ \vdots & & & & & 0 \\ \mu_{r-1} & \dots & \dots & \dots & 0 & \mu_{2r-2} \end{pmatrix} \sim \left(\begin{array}{c|c} \begin{matrix} \mu_0 & \mu_2 & \dots \\ \mu_2 & \iddots & \\ \vdots & & \end{matrix} & 0 \\ \hline 0 & \begin{matrix} \mu_2 & \mu_4 & \dots \\ \mu_4 & \iddots & \\ \vdots & & \end{matrix} \end{array}\right)$$

in the bases:

$$\left[1, x, \dots, x^{r-1}\right] \quad \rightsquigarrow \quad \left[1, x^2, \dots, x^{2(\lceil \frac{r}{2} \rceil - 1)};\ x, x^3, \dots, x^{2\lfloor \frac{r}{2} \rfloor - 1}\right]$$

Synopsis: symmetry ⇒ block diagonalisation

A quadrature provides an approximation of the definite integral of a function by a weighted sum of function values at specific *nodes*. Gaussian quadratures are constructed to yield exact results for any polynomials of degree $2r-1$ or less by a suitable choice of r nodes and weights. Cubature is a generalization of quadrature in higher dimension. □ Constructing a cubature amounts to finding a linear form $p \mapsto a_1 p(\xi_1) + \dots + a_r p(\xi_r)$ from the knowledge of its restriction to polynomials of degree d or less. The unknowns are the weights a_j and the nodes ξ_j. An approach based on moment matrices was proposed in [FP05]. With a basis-free version in terms of the Hankel operator $\mathcal{H}$ associated to a linear form, the existence of a cubature of degree d with r nodes boils down to conditions of ranks and positive semidefiniteness on $\mathcal{H}$. The nodes are recognized as the solutions of a generalized eigenvalue problem. □ Standard domains of integration are symmetric under the action of a finite group. It is natural to look for cubatures that respect this symmetry [C97]. Introducing adapted bases obtained from representation theory, the symmetry constraint allows to block diagonalize the Hankel operator $\mathcal{H}$. The size of the blocks is explicitly related to the orbit types of the nodes. From the computational point of view, we then deal with smaller-sized matrices both for securing the existence of the cubature and computing the nodes.

Hankel operator $\widehat{\mathcal{H}}$ and moment matrix H_1^B

$\Lambda : \mathbb{R}[x] \to \mathbb{R}$ linear form.

$$\widehat{\mathcal{H}} : \begin{array}{rcl} \mathbb{R}[x] & \to & \mathbb{R}[x]^* \\ f & \mapsto & \Lambda_f, \end{array} \quad \text{where} \quad \Lambda_f : \begin{array}{rcl} \mathbb{R}[x] & \to & \mathbb{R} \\ g & \mapsto & \Lambda(f\,g) \end{array}$$

If $B = \{b_1, b_2, \dots\}$ is a basis of $\mathbb{R}[x]$ then

$$H_1^B = \left(\Lambda(b_i\, b_j)\right)$$

is the matrix of $\widehat{\mathcal{H}}$ in B and B^*.

$\Pi = \ker \widehat{\mathcal{H}}$ is an ideal in $\mathbb{R}[x]$

[Curto Fialkov 96], [Laurent 05]

$\Lambda = \sum_{j=1}^{r} a_j \mathbb{1}_{\xi_j}$, with $a_j > 0$, $\xi_j \in \mathbb{R}^n$ $\quad$ iff $\quad$ $\operatorname{rank} \widehat{\mathcal{H}} = r$ $\quad$ and $\quad$ $\widehat{\mathcal{H}} \succeq 0$.

Then $\{\xi_1, \dots, \xi_r\} \subset \mathbb{R}^n$ is the variety of the ideal $\Pi = \ker \widehat{\mathcal{H}}$

Existence of a cubature of degree d with r nodes

$$H_1^B(\Lambda) = \left[\begin{array}{c} \boxed{\Omega(b_i b_j)} \\ \\ \text{rank } r \end{array}\right] \succeq 0$$

$\Lambda^{(\delta+\kappa)} : \mathbb{R}[x]_{\leq 2(\delta+\kappa)} \to \mathbb{R}$ is a *flat extension* of $\Lambda^{(\delta)} : \mathbb{R}[x]_{\leq 2\delta} \to \mathbb{R}$ if

- $\operatorname{rank} \mathcal{H}^{(\delta+\kappa)} = \operatorname{rank} \mathcal{H}^{(\delta)}$
- $\Lambda^{(\delta+\kappa)}(f) = \Lambda^{(\delta)}(f) \quad \forall f \in \mathbb{R}[x]_{\leq 2\delta}$

[Curto Fialkow 96]

If $\Lambda^{(\delta)}$ is a flat extension of its restriction $\Lambda^{(\delta-1)}$ then $\Lambda^{(\delta)}$ admits a unique flat extension $\Lambda^{(\delta+\kappa)}$ for all $\kappa \geq 1$.

Algorithm: A Gauss-Bareiss scheme *without pivoting* to obtain equations and inequalities. [Collowald, Hubert 15]

Computation of the nodes

[Brachat *et al* 10]

$\operatorname{rank} \widehat{\mathcal{H}} = r < \infty \qquad \Pi = \ker \widehat{\mathcal{H}} \qquad V(\Pi) = \{\xi_1, \dots, \xi_r\}$

$B = \{b_1, \dots, b_r\}$ is a basis of $\mathbb{R}[x]/\Pi$ iff $H_1^B = \left(\Lambda(b_i b_j)\right)$ invertible.

The eigenvalues of

$$\mathcal{M}_f : \begin{array}{rcl} \mathbb{R}[x]/\Pi & \to & \mathbb{R}[x]/\Pi \\ g & \mapsto & f\,g \end{array}$$

are $\{f(\xi_1), \dots, f(\xi_r)\}$

The matrix of $\mathcal{H} \circ \mathcal{M}_f$ is $H_f^B = \left(\Lambda(f b_i b_j)\right)$. $\qquad$ Hence $\quad M_f^B = \left(H_1^B\right)^{-1} H_f^B$

Symmetry

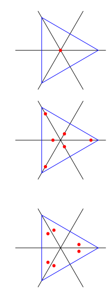
The group of isometries of the regular m-gon in the plane

$$D_m = \left\{ r^k, r^k s \mid 0 \leq k \leq m-1 \right\} \text{ with } r^m = 1,\ s^2 = 1,\ sr = r^{m-1}s$$

Irreducible representations of D_3:

	$\mathcal{R}_1$	$\mathcal{R}_2$	$\mathcal{R}_3$
s	$[1]$	$[-1]$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
r	$[1]$	$[1]$	$\begin{bmatrix} \cos(\frac{2\pi}{3}) & -\sin(\frac{2\pi}{3}) \\ \sin(\frac{2\pi}{3}) & \cos(\frac{2\pi}{3}) \end{bmatrix}$

Orbit types of the dihedral group D_3



Isotropy	Permutation representation
D_3	$\mathcal{P}_1(s) = [1], \quad \mathcal{P}_1(r) = [1]$
D_1	$\mathcal{P}_2(s) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \mathcal{P}_2(r) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$
1	$\mathcal{P}_3(s) = \begin{bmatrix} 0 & \mathcal{P}_2(s) \\ \mathcal{P}_2(s) & 0 \end{bmatrix}, \quad \mathcal{P}_3(r) = \begin{bmatrix} \mathcal{P}_2(r) & 0 \\ 0 & \mathcal{P}_2(r) \end{bmatrix}$

Matrix of multiplicities Γ_G of a finite group G

[Collowald Hubert 15]

$\mathcal{R}_1, \dots, \mathcal{R}_N$ irreducible inequivalent representations of G

$\mathcal{P}_1, \dots, \mathcal{P}_T$ permutation representation for conjugacy class of subgroups of G

$\gamma_{i,j} =$ Multiplicity of $\mathcal{R}_i$ in $\mathcal{P}_j = \langle \chi_{\mathcal{P}_j}, \chi_{\mathcal{R}_i} \rangle$

$$\Gamma_G = \left(\gamma_{i,j}\right)_{\substack{1 \leq i \leq N \\ 1 \leq j \leq T}}$$

D_3 :

$\mathcal{P}_1 \sim \mathcal{R}_1$

$\mathcal{P}_2 \sim \mathcal{R}_1 \oplus \mathcal{R}_3$

$\mathcal{P}_3 \sim \mathcal{R}_1 \oplus \mathcal{R}_2 \oplus 2\mathcal{R}_3$

$$\Gamma_{D_3} = \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \mathbf{0} & \mathbf{1} & \mathbf{2} \end{bmatrix}$$

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Invariance

$\Lambda : \mathbb{R}[x] \to \mathbb{R}$ is G-invariant if $\Lambda(g \star p) = \Lambda(p)$.

For instance $p \mapsto \int_{\triangle} p(x,y)dxdy$ is D_3 invariant.

$\Lambda = \sum_{j=1}^{r} a_j \mathbb{1}_{\xi_j}$ is G-invariant $\quad \Rightarrow \quad \{\xi_1, \dots, \xi_r\}$ is a union of orbits.

Block diagonal structure and ranks of the blocks

[Gatermann Parillo 2006], [Riener *et al.* 2011],[Collowald, Hubert 15]

$\Lambda : \mathbb{R}[x] \to \mathbb{R}$ G−invariant. In an *orthogonal symmetry adapted basis* B of $\mathbb{R}[x]_\delta$

$$H_1^B = \begin{bmatrix} H_1^{B_1} & & 0 \\ & \ddots & \\ 0 & & H_1^{B_N} \end{bmatrix} \quad \text{with} \quad H_1^{B_k} = \begin{bmatrix} H^{(k)} & & 0 \\ & \ddots & \\ 0 & & H^{(k)} \end{bmatrix}.$$

n_k identical blocks $H^{(k)}$.

[Collowald, Hubert 15]

m_ℓ number of orbits of type $\mathcal{P}_\ell$ in the set of nodes

$$\operatorname{rank} H^{(k)} = \sum_{\ell=1}^{T} \gamma_{k\ell}\, m_\ell,$$

In particular $\operatorname{rank} H^{(1)} = m_1 + \ldots + m_T$ is the number of orbits

D_6−invariant cubature of degree 13

$$\dim \left(\mathbb{R}[x]_{\leq \lfloor \frac{d}{2} \rfloor}\right)^{(k)} \leq n_k \sum_{\ell=1}^{T} \gamma_{k\ell} m_\ell \leq \dim \left(\mathbb{R}[x]_{\leq \delta - 1}\right)^{(k)}.$$

⇒ At least 37 nodes.

⇒ At least one orbit of 12 nodes

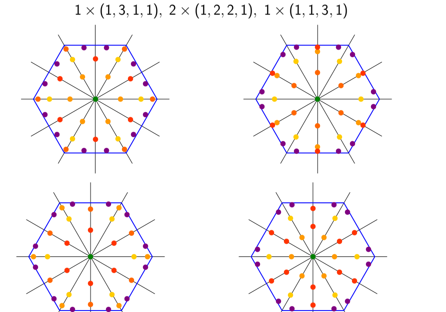
⋮

⇒ $(m_1,\ m_2,\ m_3,\ m_4) \in \{(1,3,1,1),\ (1,2,2,1),\ (1,1,3,1)\}$

[Collowald, Hubert 15]

There exist exactly 4 minimal D_6-invariant cubatures of degree 13 with 37 nodes for the hexagon.

$$1 \times (1,3,1,1),\ 2 \times (1,2,2,1),\ 1 \times (1,1,3,1)$$



D_3−invariant cubature of degree 7

Only one previously known [Laursen Gellert 78].

[Collowald Hubert 15]

For the triangle, there exist exactly two D_3-invariant cubatures of degree 7 with 1 orbit of 3 nodes and 2 orbits of six nodes.

$$m_1 = 0,\ m_2 = 1,\ m_3 = 2,\ m_4 = 0$$