Cubature formulae, flat extensions and convex relaxation.

B. Mourrain
INRIA Méditerranée, Sophia Antipolis
Bernard.Mourrain@inria.fr

(collaboration with M. Abril Bucero & C. Bajaj)

The problem

For any continuous function f, compute (an approximation of)

$$I[f] = \int_{\Omega} w(\mathbf{x}) f(\mathbf{x}) d\mathbf{x}$$

where $\Omega \subset \mathbb{R}^n$ and w is a positive function on Ω.
Cubature formula: compute $\xi_j \in \mathbb{R}^n$ and weights $w_j \in \mathbb{R}$ such that

$$\sigma : f \mapsto \langle \sigma | f \rangle = \sum_{j=1}^{r} w_j \, f(\xi_j)$$

satisfies:

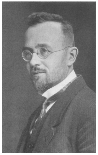
$$\langle \sigma | f \rangle = I[f], \forall f \in V,$$

where V is a finite dimensional vector space of polynomials.

Interest:

- Fast/accurate evaluation of integrals.
- Important ingredient in numerical methods.
- Applications in other domains : graph, algorithms (Lanczos), ...

A long history:

-  C.F. Gauss (1815), . . .  J. Radon (1948), W. Gröbner (1948), . . .
- A. H. Stroud (1971), I.P. Mysovskikh (1981), R. Cools (1993 ... 2003), . . .

Many case studies on simplex, hyperspheres, hypercubes, for degree 1, 2,3,4,5, . . .

Solving the cubature of the disk (cf. [Cools'00])

Table 1: Overview of published cubature formulas for the unit disk.

Degree	N	Quality	References
2	3*	PI	[25]
3	4*	PI(3)	[25]
		PB	[25]
4	6*	PI	[25]
		?O	[24]
	10	EI	[12]
5	7*	PI(2)	[25]
	8	PO	[3]
		PO	[25]
	9	PI(2)	[25]
		PB	[25]
	12	EI	[25]
		EI	[12]
		EI	[11]
6	10*	PO	[23] [26]
		PO	[18]
	11	PO	[26] [20]
	14	EI	[12]
7	12*	PI	[25]
	16	EI	[12]
		PI	[25]
	18	EI	[12]
	20	EI	[12]
8	16	PI	[20] [26]
9	18*	PO	[22]
	19	PI	[25]
		PI	[19]
		PI	[16]
		PI	[20]
	20	PI(3)	[3]
		PO	[25]
		PO	[3]
		PO	[3] [17]
	21	PI	[3]
		PI	[25]
		PO	[25]
11	25	PO	[15]
		NO	[17] Error
	26	PI	[21]
		PI	[15]
	28	PI(3)	[25]
	32	PI	[25]
13	34	PO	[9]
	35	PB	[9]
	36	PI	[7] [17]
	37	PI	[25]
	41	PI	[25]
		PI	[14]
15	44	PI	[25]
		PI	[17]
	48	PI	[25]
17	56	PO	[17] Error
	57	PI	See §3, Table 2
	60	PO	[17]
	61	PI	[25]
19	68	NO	[17] Error
	69	PO	See §3, Table 3
	71	PO	[14]
	72	PI	[17]
	76	PI	[14] [13]
21	88	PO	See §3, Table 4
	90	PI	[14]
	99	PI	[14] [4]
23	97	PO	[14]
	108	PI	[14] [13]
25	127	PI	[14]
27	140	PI	[14] [13]
31	172	PI	[14] [13]

Embedded cubature formulas

Degrees	N	Quality	References
5-7	8-16	PNI(2)	[5]
[illegible]	[illegible]	PNI	[illegible]

Example (1D)

$V = \mathbb{R}[x]_{\leq 2r-1}$ polynomials of degree $\leq 2r-1$, spanned by $1, x, \ldots, x^{2\,r-1}$.

Problem: Given $\sigma_0 = I[1], \sigma_1 = I[x], \ldots, \sigma_{2r-1} = I[x^{2r-1}]$, find $\xi_i \in \mathbb{R}$, $\omega_i \in R$ s.t.

$$\sigma_k = \sum_{i=1}^{r} \omega_i \xi_i^k. \tag{1}$$

Solution: If (1) is satisfied, then $p(x) = p_0 + p_1 x + \cdots + p_r x^r = \prod_{i=1}^{r}(x - \xi_i)$ is such that

$$\overbrace{\begin{bmatrix} \sigma_0 & \sigma_1 & \ldots & \sigma_r \\ \sigma_1 & & & \sigma_{r+1} \\ \vdots & & & \vdots \\ \sigma_{r-1} & \ldots & \sigma_{2r-1} & \sigma_{2r-1} \end{bmatrix}}^{H_\sigma} \begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_r \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{r} \omega_i p(\xi_i) \\ \sum_{i=1}^{r} \omega_i p(\xi_i)\xi_i \\ \vdots \\ \sum_{i=1}^{r} \omega_i p(\xi_i)\xi_i^{r-1} \end{bmatrix} = 0$$

☞ **Compute an element $p(x)$ in the kernel of H_σ, its roots $\xi_1, \ldots, \xi_d$ and deduce the coefficients $\omega_1, \ldots, \omega_i$ s.t. $\sigma_k = \sum_{i=1}^{d} \omega_i \xi_i^k$.**

In practice, for $\langle f, g\rangle = \sum_k \sum_{j\leq k} \sigma_k f_j g_{k-j}$,

- Compute the orthogonal polynomials $p_i(x)$ such that $\langle x^j, p_i\rangle = 0$ for $j < i$ and $\langle x^i - p_i, p_i\rangle = 0$, which satisfies the **recurrence relation**

$$p_{i+1}(x) = (x - \alpha_i)p_i(x) + \gamma_i p_{i-1}(x)$$

where $\alpha_i = \frac{\langle x\, p_i, p_i\rangle}{\langle p_i, p_i\rangle}$, $\gamma_i = \frac{\langle x\, p_i, p_{i-1}\rangle}{\langle p_{i-1}, p_{i-1}\rangle} = \frac{\langle p_i, p_i\rangle}{\langle p_{i-1}, p_{i-1}\rangle}$.

- Take the last polynomial $p(x) = p_r(x)$ for the quadrature rule.

What we are going to do

☞ Replace the cubature problem by a **low-rank structured matrix-completion problem** in a **convex set**.

☞ Relax the low-rank condition by a L_1 proxy and solve (a hierarchy of) **convex optimization problems** to obtain the minimal L_1 solutions.

☞ Deduce the **cubature formula from the completed matrix**.

- Sequences in $\mathbb{K}^{\mathbb{N}^n}$:

$$\sigma = (\sigma_\alpha)_{\alpha\in\mathbb{N}^n}$$

- Formal power series in $\mathbb{K}[[\mathbf{z}]] = \mathbb{K}[[z_1,\ldots,z_n]]$:

$$\sigma(\mathbf{z}) = \sum_{\alpha\in\mathbb{N}^n} \sigma_\alpha \frac{\mathbf{z}^\alpha}{\alpha!}$$

- Linear forms in the dual R^* where $R = \mathbb{K}[\mathbf{x}] = \mathbb{K}[x_1,\ldots,x_n]$:

$$\sigma : p = \sum_\alpha p_\alpha \mathbf{x}^\alpha \mapsto \langle\sigma|p\rangle = \sum_\alpha \sigma_\alpha p_\alpha$$

  - Isomorphism: $\mathbb{K}[\mathbf{x}]^* \sim \mathbb{K}[[\mathbf{z}_1,\ldots,\mathbf{z}_n]]$.
  - **Structure of $\mathbb{K}[\mathbf{x}]$-module:** $\forall a\in\mathbb{K}[\mathbf{x}], \forall\sigma\in\mathbb{K}[\mathbf{x}]^*$,

$$a\star\sigma : b \mapsto \langle\sigma|a\,b\rangle$$

Example:

$$x_1 \star \mathbf{z}_1^{\alpha_1}\mathbf{z}_2^{\alpha_2}\cdots\mathbf{z}_n^{\alpha_n} = \alpha_1\mathbf{z}_1^{\alpha_1-1}\mathbf{z}_2^{\alpha_2}\cdots\mathbf{z}_n^{\alpha_n} = \partial_{\mathbf{z}_1}(\mathbf{z}_1^{\alpha_1}\mathbf{z}_2^{\alpha_2}\cdots\mathbf{z}_n^{\alpha_n}).$$

Dictionary

- $p \mapsto \partial_1^{\alpha_1} \cdots \partial_n^{\alpha_n}(p)(0)$ represented by $\mathbf{z}^\alpha$.
- $p \mapsto p(\xi)$ represented by $\mathbf{e}_\xi(\mathbf{z}) = \sum_{\alpha \in \mathbb{N}^n} \xi^\alpha \frac{\mathbf{z}^\alpha}{\alpha!} = e^{\mathbf{z}\cdot\xi}$.
- $p \mapsto \int_\Omega p \, d\mu$ represented by $\sigma(\mathbf{z}) = \sum_{\alpha \in \mathbb{N}^n} \int_\Omega e^{\mathbf{x}\cdot\mathbf{z}} dx$.
- σ s.t. $\sigma_\alpha = \sum_{i=1}^r \omega_i \, {\xi_i}^\alpha$ represented by $\sigma(\mathbf{z}) = \sum_{i=1}^r \omega_i \, \mathbf{e}_{\xi_i}(\mathbf{z})$ where $\mathbf{e}_{\xi_i}(\mathbf{z}) = e^{\mathbf{z}\cdot\xi_i} = e^{z_1 \xi_{1,i} + \cdots + z_n \xi_{n,i}}$.

The cubature problem for $V = R_{\leq d}$ over $\mathbb{R}$: find

- frequencies $\xi_1, \ldots, \xi_r \in \mathbb{R}^n$,
- weights $\omega_1, \ldots, \omega_r \in \mathbb{R}$,

such that

$$\int_\Omega \mathbf{e}^{\mathbf{x}\cdot\mathbf{z}} \mathbf{dx} \equiv \sum_{\mathbf{i}=1}^{\mathbf{r}} \omega_\mathbf{i} \, \mathbf{e}_{\xi_\mathbf{i}}(\mathbf{z}) + \mathbf{O}((\mathbf{z})^{\mathbf{d}+1})$$

(Borel-Laplace transform).

Vanishing ideal, Hankel operators and moments

For $\sigma \in \mathbb{K}[\mathbf{x}]^* = \mathbb{K}[[\mathbf{z}]]$,

- **Hankel operator:**

$$\begin{array}{rcl} H_\sigma : \mathbb{K}[\mathbf{x}] & \rightarrow & \mathbb{K}[\mathbf{x}]^* \\ p & \mapsto & p \star \sigma \end{array}$$

  where $p \star \sigma : q \mapsto \langle \sigma | p\, q \rangle$.

- **Vanishing ideal:**

$$0 \rightarrow I_\sigma \rightarrow \mathbb{K}[\mathbf{x}] \rightarrow \mathcal{A}_\sigma^* \rightarrow 0$$

  with $I_\sigma := \ker H_\sigma$, $\mathcal{A}_\sigma := \mathbb{K}[\mathbf{x}]/I_\sigma$.

- **Moments** of $\sigma \in \langle \mathbf{x}^A \rangle^*$: $\langle \sigma | \mathbf{x}^\alpha \rangle \in \mathbb{K}$ for $\alpha \in A \subset \mathbb{N}^n$.
- **Truncated moment matrix:** If $E_1 = \langle \mathbf{x}^A \rangle$, $E_2 = \langle \mathbf{x}^B \rangle$, the matrix of

$$\begin{array}{rcl} H_\sigma^{E_1,E_2} : E_1 & \rightarrow & E_2^* \\ p & \mapsto & p \star \sigma \end{array} \quad \text{is the moment matrix of } [\langle \sigma | \mathbf{x}^{\alpha+\beta} \rangle]_{\alpha \in A, \beta \in B}.$$

Semi-Definite Programming Relaxation

If $\sigma = \sum_{i=1}^{r} w_j \mathbf{e}_{\xi_j}$ with $\xi_j \in \mathbb{R}^n, w_j > 0$, then $H_\sigma^{B,B} \succcurlyeq 0$ and of rank $\leq r$.

For given moments $\mathbf{i} = (\mathbf{i}(v))_{v \in V}$, consider the **convex** set:

$$\mathcal{H}^k(\mathbf{i}) \;=\; \{H_\sigma \mid \sigma \in R_{2k}^*, \forall v \in V \; \langle \sigma | v \rangle = \mathbf{i}(v), H_\sigma \succcurlyeq 0\}$$

Cubature formulae with a minimal number of points as the solution of

$$\min_{H \in \mathcal{H}^k(\mathbf{i})} \operatorname{rank}(H).$$

☞ **Relaxation of this NP-hard problem:**

$$\min_{H \in \mathcal{H}^k(\mathbf{i})} \operatorname{trace}(P^t H P) \tag{2}$$

for a well-chosen matrix P.

☞ **Optimization of a linear functional on a convex set (the cone of SDP matrices intersected with a linear space) by SDP solvers.**

Objective function: $\mathrm{trace}\,(P^t HP)$= nuclear norm of $P^t HP$.
$= \mathrm{trace}\,(HPP^t) = \langle H, Q\rangle$ where $Q = PP^t$.

Convex optimization problem:

argmin$\langle H, Q\rangle$ s.t.

- $H = (h_{\alpha,\beta})_{\alpha,\beta\in B} \succcurlyeq 0$,
- H satisfies the Hankel constraints
  $h_{\alpha,\beta} = h_{\alpha',\beta'} =: h_{\alpha+\beta}$ if $\alpha+\beta = \alpha'+\beta'$.
- $h_\alpha = I[\mathbf{x}^\alpha]$ for $\alpha \in A$.

Efficient solvers by interior point methods, with polynomial complexity (for a given precision ϵ).
Efficient tools: CSDP, SDPA, ...

Flat extension

Let $B \subset C$, $B' \subset C'$, $\partial B = C \setminus B$, $\partial B' = C' \setminus B'$.

Truncated moment matrix:

$$H^{C,C'} = \left(\langle \sigma \mid \mathbf{x}^{\alpha+\beta} \rangle \right)_{\alpha \in C, \beta \in C'}$$

Flat extension:

$$\mathbf{H}^{\mathbf{C},\mathbf{C}'} = \left[\begin{array}{c|c} \mathbf{H}^{\mathbf{B},\mathbf{B}'} & H^{B,\partial B'} \\ \hline H^{\partial B,B'} & H^{\partial B,\partial B'} \end{array} \right],$$

- $\operatorname{rank} H^{C,C} = \operatorname{rank} H^{B,B}$
- there exist $\mathbb{P} \in \mathbb{C}^{B \times \partial B'}$, $\mathbb{P}' \in \mathbb{C}^{B' \times \partial B}$ s.t.

$$\mathbb{M} = \mathbb{H}^t \, \mathbb{P}, \mathbb{M}' = \mathbb{H} \, \mathbb{P}', \mathbb{N} = \mathbb{P}^t \, \mathbb{H} \, \mathbb{P}'. \tag{3}$$

with $\mathbb{H} = H^{B,B'}$, $\mathbb{M}' = H^{B,\partial B'}$, $\mathbb{M} = H^{\partial B,B'}$, $\mathbb{N} = H^{\partial B,\partial B'}$

When there is a flat extension for $C = C' = B^+$

($B^+ = B \cup x_1 B \cup \ldots \cup x_n B$; B connected to 1)

- The tables of multiplication in $\mathcal{A}_\sigma = \mathbb{R}[\mathbf{x}]/I_\sigma$ are $M_j := H^{B,x_j B}(H^{B,B})^{-1}$.
- Their common eigenvectors $\mathbf{v_i}$ are, up to a scalar, *the* Lagrange interpolation polynomials $\mathbf{u}_{\xi_\mathbf{i}}$.
- The points of the cubature are $\xi_i = (\xi_{i,1}, \ldots, \xi_{i,n})$, where $\xi_{i,j}$ is an eigenvalue of M_j.
- The decomposition is $\sigma = \sum_{i=1}^{r} \frac{1}{\mathbf{v}_i(\xi_i)} \langle \sigma | \mathbf{v}_i \rangle \mathbf{e}_{\xi_i}$.

The geometry of $\mathcal{H}^k(\mathbf{i})$

$$
\begin{aligned}
\mathcal{H}^k(\mathbf{i}) &= \{H_\sigma \mid \sigma \in R_{2k}^*, \forall v \in V \ \langle \sigma | v\rangle = \mathbf{i}(v), H_\sigma \succcurlyeq 0\} \\
\mathcal{H}_r^k(\mathbf{i}) &= \left\{H_\sigma \in \mathcal{H}^k(\mathbf{i}) \mid \operatorname{rank} H_\sigma \leq r\right\} \\
\mathcal{E}_r^k(\mathbf{i}) &= \left\{H_\sigma \in \mathcal{H}^k(\mathbf{i}) \mid \sigma = \sum_{i=1}^{r} w_i \, \mathbf{e}_{\xi_i}, \omega_i > 0, \xi_i \in \mathbb{R}^n\right\} \\
&\subset \mathcal{H}_r^k(\mathbf{i}) \qquad\qquad \text{(cubature with r points)}
\end{aligned}
$$

Proposition

Let $k \geqslant \frac{\deg(V)+1}{2}$ and H be an element of $\mathcal{H}^k(\mathbf{i})$ with minimal rank r. If $k \geqslant r$, then $H \in \mathcal{E}_r^k(\mathbf{i})$ and it is either an extremal point of $\mathcal{H}^k(\mathbf{i})$ or on a face of $\mathcal{H}^k(\mathbf{i})$, which is included in $\mathcal{E}_r^k(\mathbf{i})$.

Remark: if σ is *interpolatory* (weights uniquely determined from the points) of minimal rank, then H_σ is **extremal**.

Theorem

Let P be a proper operator and $k \geqslant \frac{\deg(V)+1}{2}$. Assume that there exists $\sigma^* \in R^*_{2k}$ such that H_{σ^*} is a minimizer of (2) of rank r with $r \leqslant k$. Then $H_{\sigma^*} \in \mathcal{E}^k_r(\mathbf{i})$ i.e. there exists $\omega_i > 0$ and $\xi_i \in \mathbb{R}^n$ such that

$$\sigma^* \equiv \sum_{i=1}^{r} \omega_i \mathbf{e}_{\xi_i}.$$

Assume $\Omega = \{\mathbf{x} \in \mathbb{R}^n \mid g^0_1 = 0, \ldots, g^0_{n_1} = 0, g^+_1 \geq 0, \ldots, g^+_{n_2} \geq 0\}$ is compact.

Let $\mathcal{L}^k(\mathbf{i}) = \{H_\sigma \in \mathcal{H}^k(\mathbf{i}) \mid \langle \sigma \mid q\, g^0_i \rangle = 0 \text{ for } \deg(q\, g^0_i) \leq 2k, \langle \sigma \mid q^2 g^+_i \rangle \geq 0 \text{ for } \deg(q_i^2 g^+_i) \leq 2k\}$.

Theorem

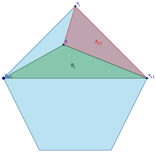
For P generic and $k \gg 0$, a minimizer H_{σ^*} of $\min_{H \in \mathcal{L}^k(\mathbf{i})} \mathrm{trace}\,(P^t H P)$ is in $\mathcal{E}^k_r(\mathbf{i})$ with $r \leqslant k$ and its associated points are in Ω.

Example (1)

Cubature on the square $\Omega = [-1, 1] \times [-1, 1]$

Degree	N	Points	Weights
3	4	±(0.46503, 0.464462)	1.545
		±(0.855875, -0.855943)	0.454996
5	7	±(0.673625, 0.692362)	0.595115
		±(0.40546, -0.878538)	0.43343
		±(-0.901706, 0.340618)	0.3993
		(0, 0)	1.14305
7	12	±(0.757951, 0.778815)	0.304141
		±(0.902107, 0.0795967)	0.203806
		±(0.04182, 0.9432)	0.194607
		±(0.36885, 0.19394)	0.756312
		±(0.875533, -0.873448)	0.0363
		±(0.589325, -0.54688)	0.50478

Example (2)



Wachpress barycentric coordinates:

- $\lambda_i(\mathbf{x}) \geq 0$ for $\mathbf{x} \in C$
- $\sum_{i=1}^{5} \lambda_i(\mathbf{x}) = 1$,
- $\sum_{i=1}^{5} v_i \cdot \lambda_i(\mathbf{x}) = \mathbf{x}$.

For $p \in R = \mathbb{R}[u_0, u_1, u_2, u_3, u_4]$,

$$I[p] = \int_{\mathbf{x} \in \Omega} p \circ \lambda(\mathbf{x}) d\mathbf{x}$$

For $B = \{1, u_0, u_1, u_2, u_3, u_4\}$, the solution of the optimization problem:

$$\begin{array}{ll} \min & \mathrm{trace}(H_\sigma^{B^+,B^+}) \\ s.t. & H_\sigma^{B^+,B^+} \succcurlyeq 0 \end{array} \qquad (4)$$

yields 5 points and weights:

Points	Weights
$(0.249888, -0.20028, 0.249993, 0.350146, 0.350193)$	0.485759
$(0.376647, 0.277438, -0.186609, 0.20327, 0.329016)$	0.498813
$(0.348358, 0.379898, 0.244967, -0.174627, 0.201363)$	0.509684
$(-0.18472, 0.277593, 0.376188, 0.329316, 0.201622)$	0.490663
$(0.242468, 0.379314, 0.348244, 0.200593, -0.170579)$	0.51508

Open questions:

- Optimal choice of the matrix P for minimal rank r.
- Control the order k of relaxation.
- Numerical best rank r approximation for sparse representation.
- Low rank structured matrix completion problem.

Thank you for your attention