

OPTIMAL GAUSSIAN QUADRATURE

ABSTRACT. Classical Gaussian quadrature is anchored in the space of real polynomials at polynomial degree 0 and is monotonically directed by successively increasing polynomial degree. Recent research, showing that it's possible to weigh anchor and chart various courses in search of the best currents in the superspace of real Laurent polynomials, is presented.

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FURTHER READING

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October, 2009

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Theorem 0.1. ([1] Theorem 3.13) Let $\langle \{z^{p(n)}\}_{n=1}^k \rangle$ be the Laurent polynomial space over \mathbb{F} with order implied by ordered basis $A = \{z^{p(n)}\}_{n=1}^k$ for some $k \in \mathbb{N} \cup [\infty]$ and injection $p : [n \in \mathbb{N} : 1 \leq n < k + 1] \rightarrow \mathbb{Z}$. Let $\mathcal{L} : \Omega \rightarrow \mathbb{C}$ be a strong moment functional, moments $\mu_n = \mathcal{L}(z^n)$, $n \in \mathbb{Z}$. Then:

(A) $R \cdot S = \mathcal{L}(RS)$ is an inner product on $\langle \{z^{p(n)}\}_{n=1}^k \rangle$ over \mathbb{F} if and only if

$$(0.1a) \quad \mathbb{F} \text{ is a subfield of } \mathbb{R},$$

$$(0.1b) \quad \mu_{p(i)+p(j)} \in \mathbb{F} \text{ for all } i, j \text{ such that } 1 \leq i, j < k + 1,$$

and

$$(0.1c) \quad \text{for all } m \text{ such that } 1 \leq m < k + 1,$$

$$|G_m| := \begin{vmatrix} \mu_{p(1)+p(1)} & \mu_{p(1)+p(2)} & \cdots & \mu_{p(1)+p(m)} \\ \mu_{p(2)+p(1)} & \mu_{p(2)+p(2)} & \cdots & \mu_{p(2)+p(m)} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{p(m)+p(1)} & \mu_{p(m)+p(2)} & \cdots & \mu_{p(m)+p(m)} \end{vmatrix} > 0.$$

(B) If $\mathbb{F} = \mathbb{R}$ and p is a bijection from \mathbb{N} to \mathbb{Z} , then $\langle \{z^{p(n)}\}_{n=1}^k \rangle$ is the space

$$A^{\mathbb{R}} := \left[\sum_{i=m}^n r_i x^i : m, n \in \mathbb{Z}, r_i \in \mathbb{R} \text{ for } m \leq i \leq n \right]$$

of all real Laurent polynomials, and the following conditions are equivalent:

(I) $\mathcal{L}(S^2) > 0$ for all non-zero S in $A^{\mathbb{R}}$.

(II) (0.1c) with $k = \infty$ holds.

(III) $\mathcal{L}(R) > 0$ for all non-zero R in $A^{\mathbb{R}}$ such that $R(x) \geq 0$ for all $x \in \mathbb{R}^* := \mathbb{R} - [0]$ (i.e., \mathcal{L} is positive definite).

Furthermore, (I)-(III) are implied by the condition

(SMDF) $\mathcal{L}(Q) = \int_{\mathbb{R}^*} Q(x) d\phi(x)$ for some $\phi \in \Phi$ and all Q in $A^{\mathbb{R}}$.

(C) If (0.1) holds, then $\{Q_n(x)\}_{n=1}^k$ such that $|G_0| := 1$ and

$$(0.2) \quad Q_n(x) = |G_{n-1}|^{-1} \begin{vmatrix} \mu_{p(1)+p(1)} & \cdots & \mu_{p(1)+p(n-1)} & x^{p(1)} \\ \vdots & & \vdots & \vdots \\ \mu_{p(n)+p(1)} & \cdots & \mu_{p(n)+p(n-1)} & x^{p(n)} \end{vmatrix}$$

is the monic OLPS in $\langle \{x^{p(n)}\}_{n=1}^k \rangle$ with respect to the inner product $R \cdot S = \mathcal{L}(RS)$ and ordered basis $A = \{x^{p(n)}\}_{n=1}^k$.

Theorem 0.2. ([1] Theorem 5.1) Let $\{\mathcal{A}_n\}_{n=1}^k$ be an OLPS with respect to an inner product \cdot on an L space V . Let rank ρ and leading coefficient κ of elements of V be relative to $\{\mathcal{A}_n\}_{n=1}^k$. Then:

$\{\mathcal{A}_n\}_{n=1}^k$ satisfies the system of three-term recurrence relations

$$(0.3a) \quad \mathcal{A}_{-1} := 1, \mathcal{A}_0 := 0, \text{ and } \mathcal{A}_n = b_n \mathcal{A}_{n-1} + a_n \mathcal{A}_{n-2} \text{ for } 1 \leq n < k + 1$$

where

$$(0.3b) \quad b_n := q_n - \frac{(q_n \mathcal{A}_{n-1}) \cdot \mathcal{A}_{n-1}}{\mathcal{A}_{n-1} \cdot \mathcal{A}_{n-1}} \text{ for } n \geq 2,$$

$$(0.3c) \quad a_1 := \mathcal{A}_1, \text{ and } a_n := -\frac{(q_n \mathcal{A}_{n-1}) \cdot \mathcal{A}_{n-2}}{\mathcal{A}_{n-2} \cdot \mathcal{A}_{n-2}} \neq 0 \text{ for } n \geq 3$$

(a_2 and b_1 are free)

if and only if, for all n such that $2 \leq n < k + 1$, $\rho(q_n \mathcal{A}_{n-1}) = n$, $\kappa(q_n \mathcal{A}_{n-1}) = 1$, $(q_n \mathcal{A}_{n-1}) \cdot \mathcal{A}_{n-2} \neq 0$ if $n \geq 3$, and $(q_n \mathcal{A}_{n-1}) \cdot \mathcal{A}_j = 0$ if $1 \leq j \leq n - 3$.

Features of Block-Formed OLPS Examples for a Hermite PDSMF.

Example 1. $A = \{1, x, x^2, x^3, x^4, x^5, x^6\}$ $\mathcal{L}[r(x)] = \int_{-\infty}^{\infty} r(x) e^{-(x-1/x)^2} dx$

Rank	Monic OLPS Member	$p(A, \rho)$	$Q_\rho(x)/x^{p(A, \rho)}$
ρ	$Q_\rho(x)$		
1	1	0	1
2	x	0	x
3	$\frac{-3}{2} + x^2$	0	$\frac{-3}{2} + x^2$
4	$\frac{-13x}{6} + x^3$	0	$\frac{-13x}{6} + x^3$
5	$\frac{31}{8} - \frac{19x^2}{4} + x^4$	0	$\frac{31}{8} - \frac{19x^2}{4} + x^4$
6	$\frac{877x}{124} - \frac{193x^3}{31} + x^5$	0	$\frac{877x}{124} - \frac{193x^3}{31} + x^5$
7	$\frac{-865}{61} + \frac{5967x^2}{244} - \frac{603x^4}{61} + x^6$	0	$\frac{-865}{61} + \frac{5967x^2}{244} - \frac{603x^4}{61} + x^6$

Example 2. $A = \{1, \frac{1}{x}, x, \frac{1}{x^2}, x^2, \frac{1}{x^3}, x^3\}$

1	1	0	1
2	$\frac{1}{x}$	0	$\frac{1}{x}$
3	$\frac{-1}{x} + x$	-1	$-1 + x^2$
4	$\frac{1}{x^2} - 1$	1	$\frac{1}{x^3} - \frac{1}{x}$
5	$\frac{1}{x^2} - \frac{5}{2} + x^2$	-2	$1 - \frac{5x^2}{2} + x^4$
6	$\frac{1}{x^3} - \frac{5}{2x} + x$	2	$\frac{1}{x^5} - \frac{5}{2x^3} + \frac{1}{x}$
7	$\frac{-1}{x^3} + \frac{9}{2x} - \frac{9x}{2} + x^3$	-3	$-1 + \frac{9x^2}{2} - \frac{9x^4}{2} + x^6$

Example 3. $A = \{\frac{1}{x}, \frac{1}{x^2}, 1, \frac{1}{x^3}, \frac{1}{x^4}, x, \frac{1}{x^5}, \frac{1}{x^6}, x^2\}$

1	$\frac{1}{x}$	-1	1
2	$\frac{1}{x^2}$	-1	$\frac{1}{x}$
3	$\frac{-2}{3x^2} + 1$	-2	$\frac{-2}{3} + x^2$
4	$\frac{1}{x^3} - \frac{3}{2x}$	0	$\frac{1}{x^3} - \frac{3}{2x}$
5	$\frac{1}{x^4} - \frac{7}{2x^2} + 2$	0	$\frac{1}{x^4} - \frac{7}{2x^2} + 2$
6	$\frac{1}{2x^3} - \frac{7}{4x} + x$	-4	$\frac{x}{2} - \frac{7x^3}{4} + x^5$
7	$\frac{1}{x^5} - \frac{6}{x^3} + \frac{33}{4x} - \frac{5x}{2}$	1	$\frac{1}{x^6} - \frac{6}{x^4} + \frac{33}{4x^2} - \frac{5}{2}$
8	$\frac{1}{x^6} - \frac{39}{5x^4} + \frac{291}{20x^2} - \frac{61}{10}$	1	$\frac{1}{x^7} - \frac{39}{5x^5} + \frac{291}{20x^3} - \frac{61}{10x}$
9	$\frac{6}{53x^6} - \frac{68}{53x^4} + \frac{429}{106x^2} - \frac{423}{106} + x^2$	-6	$\frac{6}{53} - \frac{68x^2}{53} + \frac{429x^4}{106} - \frac{423x^6}{106} + x^8$

Lemma 0.3. *(In [2]) If $\{Q_n(x)\}_{n=1}^k$ for some $k \in \mathbb{N} \cup [\infty]$ is an OLPS with respect to a PDSMF and ordered basis of the form $\{x^{p+(n-1)}\}_{n=1}^k$ or $\{x^{p-(n-1)}\}_{n=1}^k$ for some $p \in \mathbb{Z}$, then $Q_n(x)/x^p$ has $n - 1$ simple zeros in $\mathbb{R} \cup [\infty]$ for each index n ; i.e., $\{Q_n(x)\}_{n=1}^k$ is strongly regular.*

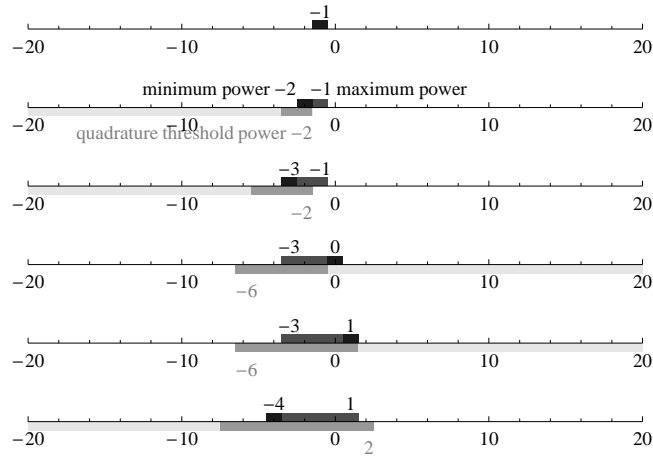
Proof. Without loss of generality, assume $\{Q_n(x)\}_{n=1}^k$ is monic. Take $q_n = x$ in the case of ordered basis $\{x^{p+(n-1)}\}_{n=1}^k$ or $q_n = 1/x$ in the case of $\{x^{p-(n-1)}\}_{n=1}^k$, and apply Theorem 0.2 to show $\{Q_n(z)\}_{n=1}^k$ satisfies a system of three-term recurrence of the form (0.3). Hence, $\{Q_n(x)/x^p\}_{n=1}^k$ also satisfies that system, and the canonical proof for orthogonal polynomial sequences (the case with ordered basis $\{1, x, x^2, \dots\}$) can be adapted to finish the proof. \square

Remark 0.4. To apply Theorem 0.2 in the previous proof, one needs to verify $(q_n Q_{n-1}) \cdot Q_{n-2} \neq 0$ if $n \geq 3$ and $(q_n Q_{n-1}) \cdot Q_j = 0$ if $1 \leq j \leq n - 3$, both of which depend on the form of the inner product; in particular, for L-polynomials R and S , $(q_n R) \cdot S = \mathcal{L}[(q_n R)S] = \mathcal{L}[R(q_n S)] = R \cdot (q_n S)$, and $(q_n Q_{n-1}) \cdot Q_{n-2} = Q_{n-1} \cdot (q_n Q_{n-2}) = Q_{n-1} \cdot Q_{n-1} = \mathcal{L}[Q_{n-1}^2] > 0$ since \mathcal{L} is positive definite.

Proposition 0.5. *(In [2]) Every block-formed OLPS with respect to a PDSMF is strongly regular.*

Power Blocks for an Example Block-formed Basis A .

$$A = \{1/x, 1/x^2, 1/x^3, 1, x, 1/x^4\}$$



KEY: Top to bottom, the graphs correspond to rank n in A , from 1 to 6.

- [*black box*] The power $p(n)$
- [*dark gray block*] The set $[p(1), \dots, p(n-1)]$
- [*medium gray block*] The exact power block at rank n in A
- [*light gray block*] The strongly regular power ray, without the exact power block, at rank n in A

Block-formed Quadrature Error for a Legendre PDSMF \mathcal{L} and an Example Block-formed Basis A .

$$\mathcal{L}[r(x)] = \int_1^2 r(x) dx \quad A = \{1/x, 1/x^2, 1/x^3, 1, x, 1/x^4\}$$

p	$E_2[x^p]$	$E_3[x^p]$	$E_4[x^p]$	$E_5[x^p]$	$E_6[x^p]$
-10	0.0608376	0.00404942	0.00013516	7.65131×10^{-6}	8.87307×10^{-8}
-9	0.0577698	0.00263129	0.0000597542	2.80509×10^{-6}	2.00427×10^{-8}
-8	0.0527518	0.00147776	0.0000199477	7.58417×10^{-7}	2.48019×10^{-9}
-7	0.0454102	0.000651042	3.83158×10^{-6}	1.14571×10^{-7}	0.0
-6	0.0355469	0.000173611	0.0	0.0	0.0
-5	0.0234375	0.0	0.0	0.0	0.0
-4	0.0104167	0.0	0.0	0.0	0.0
-3	0.0	0.0	0.0	0.0	0.0
-2	0.0	0.0	0.0	0.0	0.0
-1	0.0264805	0.000839488	0.0	0.0	0.0
0	0.111111	0.00591716	0.0000372094	0.0	0.0
1	0.314815	0.0252617	0.000371108	0.0	0.0
2	0.753086	0.0846726	0.00213055	2.36745×10^{-6}	0.0
3	1.643	0.245533	0.00924083	0.0000307261	1.02603×10^{-7}
4	3.39067	0.646696	0.0336424	0.000222849	1.63081×10^{-6}

Block-formed Quadrature Error (in [3]):

$$(0.5) \quad \mathcal{E}_n[r(x)] := \mathcal{L}[r(x)] - \mathcal{Q}[r(x)].$$

$$\mathcal{Q}[r(x)] := \sum_{i=1}^{\nu_n} r(t_{n,i}) \lambda_{n,i}$$

where $t_{n,i}$ are the non-zero, simple real zeros of $Q_n(x)$

$$\text{and } \lambda_{n,i} = \mathcal{L} \left[\left(\frac{x}{t_{n,i}} \right)^{p(A,n)+(1-d(n))/2} \frac{Q_n(x)}{(x-t_{n,i})Q'_n(t_{n,i})} \right].$$

KEY: *error numbers* Numerical values, Formula (0.4) or (0.5)
 [medium gray block] The exact power block at rank n in A
 [light gray block] The strongly regular power ray, without
 the exact power block, at rank n in A

Block-formed Quadrature Error for a Hermite PDSMF \mathcal{L} and an Example Block-formed Basis A .

$$\mathcal{L}[r(x)] = \int_{-\infty}^{\infty} r(x) e^{-(x-1/x)^2} dx \quad A = \{1/x, 1/x^2, 1/x^3, 1, x, 1/x^4\}$$

p	$\mathcal{E}_2[x^p]$	$\mathcal{E}_3[x^p]$	$\mathcal{E}_4[x^p]$	$\mathcal{E}_5[x^p]$	$\mathcal{E}_6[x^p]$
-10	65.47	56.497	56.497	25.0359	25.0359
-9	0.0	0.0	0.0	0.0	0.0
-8	17.0599	11.0778	11.0778	2.21557	2.21557
-7	0.0	0.0	0.0	0.0	0.0
-6	5.76048	1.77245	1.77245	0.0	0.0
-5	0.0	0.0	0.0	0.0	0.0
-4	2.65868	0.0	0.0	0.0	0.0
-3	0.0	0.0	0.0	0.0	0.0
-2	1.77245	0.0	0.0	0.0	0.0
-1	0.0	0.0	0.0	0.0	0.0
0	1.77245	0.590818	0.590818	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0
2	2.65868	1.87092	1.87092	0.443113	0.443113
3	0.0	0.0	0.0	0.0	0.0
4	5.76048	5.2353	5.2353	2.76946	2.76946

(In [3]) For each natural number n ,

$$\mathcal{L}[r(x)] = \sum_{i=1}^{\nu_n} r(t_{n,j}) \lambda_{n,i} \text{ for all } r(x) \in \langle \{x^{2p(A,n)+d(n)\times(i-1)}\}_{i=n-\nu_n}^{2n-2} \rangle.$$

KEY: *error numbers* Numerically derived values using Formula (0.5)
[medium gray block] The exact power block for special Quadrature with 0 error by Formula (0.4)

Proposition 0.6. (In [4].) Suppose \mathcal{L} is a PDSMF of the form

$$\mathcal{L}[f(x)] = \int_a^b f(x) w(x) dx,$$

corresponding to a continuous, non-negative weight function $w(x)$ on an interval $[a, b] \subset \mathbb{R}^*$. Then, for each rank n , any block-formed orthogonal Laurent polynomial $Q_n(x)$ has $\nu_n = n - 1$ simple zeros in the open interval (a, b) .

Proof. $Q_1(x) = x^{p(1)}$ has no zeros in (a, b) since this interval does not contain 0 or ∞ . Now, let rank n be greater than 1, and adapt the canonical path to proof for the polynomial case as follows. By orthogonality, $\mathcal{L}[x^{p(A,n)}Q_n(x)] = 0$, which implies $Q_n(x)$ must change sign at least once in (a, b) , hence $Q_n(x)$ has at least one zero of odd multiplicity in (a, b) . Let $q(x) = \prod_{i=1}^j (x - x_i^{d(n)})$ where x_i for $1 \leq i \leq j$ denote the distinct zeros of odd multiplicity of $Q_n(x)$ in (a, b) . Then $x^{p(A,n)}q(x^{d(n)})Q_n(x)$ is an L-polynomial that has no zeros in (a, b) of odd multiplicity, hence one finds $x^{p(A,n)}q(x^{d(n)})Q_n(x) \geq 0$ for all x in (a, b) . It follows that $\mathcal{L}[x^{p(A,n)}q(x^{d(n)})Q_n(x)] > 0$. If the degree j of $q(x)$ is less than $n - 1$, then $x^{p(A,n)}q(x^{d(n)})$ is in the linear span of $\{x^{p(i)}\}_{i=1}^{n-1}$, and it would follow that $\mathcal{L}[x^{p(A,n)}q(x^{d(n)})Q_n(x)]$ is zero, contradicting $\mathcal{L}[x^{p(A,n)}q(x^{d(n)})Q_n(x)] > 0$. Hence, $j \geq n - 1$. But $Q_n(x)$ has at most $n - 1$ distinct zeros in \mathbb{R}^* in total, hence $j = n - 1$, which completes the proof. \square

Quadratures $\mathcal{Q}_n[r(x)]$ and Corresponding Standard Error Bounds $\mathcal{B}_n[r(x)]$, Varying by Block-formed Basis A .

$$\mathcal{L}[r(x)] = \int_1^2 r(x) dx \quad r(x) = 1$$

$$\mathcal{B}_n[r(x)] := \frac{1}{(2(n-1))!} (\max_{\xi \in [a,b]} |R^{(2(n-1))}(\xi)|) \int_a^b Q_n^2(x) dx$$

where $R(x) := r(x^{d(n)})/x^{2[d(n) \times p(A,n)]}$ is in $C^{2(n-1)}[a, b]$.

A	$\mathcal{Q}_2[r(x)]$	$\mathcal{B}_2[r(x)]$	$\mathcal{Q}_5[r(x)]$	$\mathcal{B}_5[r(x)]$
$\{\frac{1}{x^5}, \frac{1}{x^4}, \frac{1}{x^6}, \frac{1}{x^7}, \frac{1}{x^3}\}$	0.353123	22.3431	0.997564	0.022103
$\{x^3, x^4, x^5, x^2, x\}$	0.616934	16.3152	0.999957	0.000353435
$\{\frac{1}{x^3}, \frac{1}{x^2}, \frac{1}{x^4}, \frac{1}{x^5}, \frac{1}{x}\}$	0.607098	1.95565	0.999953	0.0000941398
$\{\frac{1}{x^4}, \frac{1}{x^3}, \frac{1}{x^2}, \frac{1}{x}, 1\}$	0.456672	6.90079	0.999999	1.11321×10^{-6}
$\{x, x^2, x^3, x^4, 1\}$	0.903374	0.519643	0.999999	1.046×10^{-6}
$\{\frac{1}{x^3}, \frac{1}{x^2}, \frac{1}{x}, 1, x\}$	0.607098	1.95565	1.0	0.0
$\{\frac{1}{x^2}, \frac{1}{x}, 1, x, x^2\}$	0.797012	0.428571	1.0	0.0
$\{x, 1, x^2, x^3, x^4\}$	0.964286	0.0357143	1.0	0.0
$\{1, \frac{1}{x}, \frac{1}{x^2}, x, \frac{1}{x^3}\}$	1.0	0.0	1.0	0.0