COMPUTATIONAL STUDIES IN ANCHORLESS UNIVERSAL STEERING OF STRONG GAUSSIAN QUADRATURE

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ABSTRACT. As described by the author in previous articles, algorithms referred to as Anchorless Universal Steering seek to obtain values of the trailing power $p \in \mathbb{Z}$ and direction $d \in \{\pm 1\}$ that minimize the norm $\|Q_n\|_{\mathcal{L}}$ of the monic ordered orthogonal Laurent polynomial $Q_n(x)$ of rank n corresponding to p, d, and positive definite strong moment functional \mathcal{L} . In this article, numerical results of a survey of Anchorless Universal Steering for various positive definite strong moment functionals are presented.

1. Introduction

An orthogonal Laurent polynomial sequence (OLPS) is an ordered orthogonal basis for an inner product space whose elements are Laurent polynomials, finite linear combinations over a subfield of the complex numbers of the integer powers of a variable z, although it is conventional to use x when over the real numbers. For example, a real orthogonal polynomial sequence is an OLPS, ordered by polynomial degree with standard ordered basis $\{1, x, x^2, \dots\}$.

In general, given an inner product, one is free to choose an ordered basis from which an OLPS can be constructed using the Gram-Schmidt orthogonalization process. The present article chronicles the results of investigations into the advantages to be gained by judicious choice of ordered basis for improving the Gaussian quadrature associated with the OLPS.

The mathematical notations, formulations, and basic theory of block-formed quadrature introduced in [2] and continued in [3] provides the starting point for the exposition here and traces back through [1], [5], and the work of Njåstad and Thron around 1980 rooted in strong moment problems and published in [6].

To begin a summary of the exposition in [2] pertinent to our purposes, given an initial integer power p(1) (anchoring) and a sequence $d: \mathbb{N} \to \{-1,1\}$ of directions (steering), a unique block-formed ordered basis $A = \{x^{p(n)}\}_{n=1}^{\infty}$ spanning a subspace of the space of all real Laurent polynomials is specified recursively by the power sequence

$$(1.1a) \qquad p(n) := \begin{cases} p(1), & \text{if } n = 1 \\ \max[p(j): 1 \le j \le n-1] + 1, & \text{if } n > 1 \text{ and } d(n) = 1 \\ \min[p(j): 1 \le j \le n-1] - 1, & \text{if } n > 1 \text{ and } d(n) = -1 \end{cases}.$$

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It is convenient to utilize the trailing power at rank n which may be defined by

(1.1b)
$$p(A,n) := \begin{cases} \min[p(j) : 1 \le j \le n], & \text{if } d(n) = 1\\ \max[p(j) : 1 \le j \le n], & \text{if } d(n) = -1 \end{cases}.$$

As a basis for more general cases of interest, attention is initially focused on positive definite strong moment functionals (PDSMFs) \mathcal{L} of the form

(1.2)
$$\mathcal{L}[r(x)] = \int_a^b r(x) \ w(x) \, dx$$

corresponding to continuous, non-negative weight functions w(x) on intervals $[a, b] \subset \mathbb{R}^*$, the set of non-zero real numbers.

Using the real inner product induced by \mathcal{L} , the Gram-Schmidt orthogonalization process produces the unique monic OLPS $\{Q_n(x)\}_{n=1}^{\infty}$ with respect to block-formed ordered basis A and PDSMF \mathcal{L} , and $\{Q_n(x)\}_{n=1}^{\infty}$ itself is called block-formed. When \mathcal{L} is of integral form (1.2), any rank n block-formed OLPS member $Q_n(x)$ is guarantied to have exactly n-1 simple zeros in (a,b).

For our quadrature purposes, the Christoffel numbers are given by

(1.3a)
$$\lambda_{n,i} := \mathcal{L}\left[\left(\frac{x}{t_{n,i}}\right)^{p(A,n)+(1-d(n))/2} \frac{Q_n(x)}{(x-t_{n,i})Q'_n(t_{n,i})}\right], i = 1, \dots, n-1,$$

for the distinct zeros $t_{n,i}$ of $Q_n(x)$. The block-formed (Gaussian) quadrature of rank n in A for \mathcal{L} is

(1.3b)
$$Q_n[r(x)] := \sum_{i=1}^{n-1} r(t_{n,i}) \lambda_{n,i},$$

and the corresponding block-formed quadrature error is

(1.3c)
$$\mathcal{E}_n[r(x)] := \mathcal{L}[r(x)] - \mathcal{Q}_n[r(x)];$$

in summary, for each natural number n,

$$\mathcal{L} = \mathcal{Q}_n + \mathcal{E}_n$$

for all r(x) defined on [a, b] such that $\mathcal{L}[r(x)]$ exists.

Theorem 1.1. (Block-formed Quadrature, [2]) Let n be any rank and $[a,b] \subset \mathbb{R}^*$. If w(x) is a continuous, non-negative weight function on the interval [a,b] and $r(x) \in C^{2(n-1)}[a,b]$, the space of all functions with 2(n-1) continuous derivatives on [a,b], then

(1.4a)
$$\int_{a}^{b} r(x) \ w(x) dx = \sum_{i=1}^{n-1} r(t_{n,i}) \lambda_{n,i} + \mathcal{E}_{n}[r(x)]$$

where $t_{n,1}, t_{n,2}, \ldots, t_{n,n-1}$ denote the non-zero simple real zeros of the monic block-formed OLPS member $Q_n(x)$, the Christoffel numbers $\lambda_{n,1}, \lambda_{n,2}, \ldots, \lambda_{n,n-1}$ are given by Formula (1.3a), and the block-formed quadrature error is given by

(1.4b)
$$\mathcal{E}_n[r(x)] = \frac{R_n^{(2(n-1))}(\xi)}{(2(n-1))!} \int_a^b Q_n^2(x) w(x) dx \text{ for some } \xi \in (a,b)$$

with
$$R_n(x) := r(x^{d(n)})/x^{2[p(A,n)\times d(n)]}$$
.

Remark 1.2. With

$$||Q_n||_{\mathcal{L}} := \left(\int_a^b Q_n^2(x) \, w(x) \, dx\right)^{1/2}$$

denoting the L² norm of Q_n with respect to \mathcal{L} , Formula (1.4b) is written as $\mathcal{E}_n[r(x)] = \frac{R_n^{(2(n-1))}(\xi)}{(2(n-1))!} \|Q_n\|_{\mathcal{L}}^2$.

Under the hypotheses of Theorem 1.1, it follows that the order 2(n-1) derivative of $R_n(x) := r(x^{d(n)})/x^{2[p(A,n)\times d(n)]}$ is continuous on [a,b], and hence

(1.5)
$$\mathfrak{B}_n[r(x)] := \frac{1}{(2(n-1))!} \left(\max_{x \in [a,b]} |R_n^{(2(n-1))}(x)| \right) ||Q_n||_{\mathcal{L}}^2$$

exists. \mathfrak{B}_n is the standard error bound at rank n, and clearly

$$(1.6) |\mathcal{E}_n[r(x)]| \le \mathfrak{B}_n[r(x)] for all r(x) \in C^{2(n-1)}[a,b].$$

It can be seen from error formula (1.4b) and was reported in [2] that

(1.7)
$$\mathcal{E}_n[r(x)] = 0 \text{ for all } r(x) \in \langle \{x^{2p(A,n)+d(n)\times(i-1)}\}_{i=1}^{2n-2} \rangle;$$

in other words, the quadrature formula (1.4a) is exact for all Laurent polynomials in the real linear span of $\{x^{2p(A,n)+d(n)\times(i-1)}\}_{i=1}^{2n-2}$, hence delivers exactness on the maximum subspace dimension of 2(n-1) at each rank n.

In the polynomial case with $A = \{1, x, x^2, \dots\}$, (1.3) through (1.7) resolve to the canonical results from classical Gaussian quadrature, and results like (1.6) and (1.7) beg a central question:

(*) Which choice of anchoring and steering gives the *optimal* rank n Gaussian quadrature for the numerical evaluation of $\mathcal{L}[r(x)]$?

Many considerations enter into the debate about how to assess quadrature optimality. This author, in [3], introduced a selection of algorithms and cost estimates and investigated the following choice in the pursuit of answering (*) with consideration of performance and expense:

(**) An optimal rank n Gaussian quadrature for the numerical evaluation of $\mathcal{L}[r(x)]$ is one with the lowest product of computing cost and standard error bound $\mathfrak{B}_n[r(x)]$.

The key observation for algorithms studied in [3] is that $Q_n(x)$, hence the rank n quadrature and error bounds $\mathfrak{B}_n[r(x)]$, is uniquely determined by n, d, and p. In terms of Gram matrix determinants,

(1.8a)
$$||Q_n||_{\mathcal{L}}^2 = \frac{|G_n(d(n), p(A, n))|}{|G_{n-1}(d(n), p(A, n))|}$$

where $|G_m(d(n), p(A, n))| :=$

$$\begin{vmatrix} \mu_{2p(A,n)} & \mu_{2p(A,n)+d(n)} & \cdots & \mu_{2p(A,n)+(m-1)d(n)} \\ \mu_{2p(A,n)+d(n)} & \mu_{2p(A,n)+2d(n)} & \cdots & \mu_{2p(A,n)+md(n)} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{2p(A,n)+(m-1)d(n)} & \mu_{2p(A,n)+md(n)} & \cdots & \mu_{2p(A,n)+(m+m-2)d(n)} \end{vmatrix}$$

for strong moments $\mu_k := \mathcal{L}[x^k]$, $k \in \mathbb{Z}$. To minimize $\mathfrak{B}_n[r(x)]$, it suffices to minimize the product of (1.8a) and

$$(1.8b) \qquad \max_{x \in [a,b]} |R_n^{(2(n-1))}(x)| = \max_{x \in [a,b]} \left| \frac{d^{2(n-1)}}{dx^{2(n-1)}} \left(r(x^{d(n)}) / x^{2[p(A,n) \times d(n)]} \right) \right|.$$

And, for the monic OLPS member $Q_n(x)$,

$$(1.9) \quad |G_{n-1}(d(n), p(A, n))| \ Q_n(x) = \left| \begin{array}{cccc} \mu_{2p(A, n)} & \cdots & \mu_{2p(A, n) + (n-2)d(n)} & x^{p(A, n)} \\ \vdots & & \vdots & & \vdots \\ \mu_{2p(A, n) + (n-1)d(n)} & \cdots & \mu_{2p(A, n) + (n+n-3)d(n)} & x^{p(A, n) + (n-1)d(n)} \end{array} \right|.$$

As described in [3], anchorless steering algorithms seek to find values for trailing power p(A, n) and direction d(n) at each rank n, not depending on earlier ranks, which minimize a compass measurement. The compass values can be determined using information regarding the rank n, the PDSMF \mathcal{L} , and the integrand r(x). When (1.8a) is used without information about the integrand r(x) in determining the compass value, the algorithm has been called Anchorless Universal Steering, and when (1.8b) is used without regard to \mathcal{L} , the algorithm has been referred to as Anchorless Existential Steering. As far as performance is concerned as gauged by the magnitude of the standard error bound, Anchorless SEBM (standard error bound minimization) Steering which minimizes the product of (1.8a) and (1.8b) is best of the three. However, Anchorless SEBM Steering has relatively high associated computing costs which can swing the optimality balance in favor of other choices, including Anchorless Universal Steering, the focus of the numerical survey reported in the section below.

2. Numerical Survey Results

Plots below in the figures are base 10 logarithms of min $\{\|Q_n\|_{\mathcal{L}}^2: d=\pm 1\}$ as a function of rank n and trailing power p, smoothly interpolated between the input points (n,p) in $\mathbb{N} \times \mathbb{Z}$. The logarithm and interpolation are being applied only for the purposes of improved topographical relief.

Figure 1 displays numerical confirmation for a Legendre-type PDSMF \mathcal{L} in which the rank n Universal Steering compass measure $\|Q_n\|_{\mathcal{L}}^2$ has no global minimum as a function of direction d and trailing power p. It is easily seen considering $\mathcal{L}[r(x)] = \int_1^2 r(x) \, dx$ that, at fixed n and p, the compass value is less with d = -1 than with d = 1, and, with d = -1 and fixed n, $\|Q_n\|_{\mathcal{L}}^2$ decreases monotonically to 0 as p tends to $-\infty$.

Figures 2 through 5 show a variety of exponential weight functions on the positive reals of the form $w(x) = e^{-x^{\beta}-1/x^{\alpha}}$ for parameters $\alpha, \beta \in \{1, 2\}$. It is a technical exercise to extend results like the Block-formed Quadrature Theorem 1.1 to cases beyond those with support on closed and bounded intervals [a, b] in \mathbb{R}^* , like those numerically explicated in all the remaining figures starting with Figure 2. In any case, all standard error bounds like (1.5) include the factor $||Q_n||_{\mathcal{L}}^2$, the compass measure for Universal Steering.

Figure 6 features a change in compass directions from d=1 at rank n=3 to d=-1 at rank n=4 in the case corresponding to weight function $w(x)=\min\left(e^{-1-1/x},e^{-x-1/x}\right)$ on $(0,\infty)$.

Figures 7 through 11 display case studies corresponding to strong moment functional analogues of the classical distributions of Hermite, Legendre, Tchebycheff, Laguerre, and Poisson types, respectively. These analogues were derived using the doubling transformation $x \to \frac{1}{\lambda}(x-\gamma/x)$ of parameters $\gamma, \lambda > 0$ as studied in the mid-1990's by Hagler, Jones, and Thron, and have appeared in journal articles beginning with [4]. All in this group of examples were chosen with $\gamma = \lambda = 1$, including the final study whose results are shown in Figure 11 for a discrete case obtained by applying the doubling transformation to a Poisson cumulative distribution function with jumps of length $\frac{1}{k!}$ at $k = 0, 1, 2, \ldots$

3. Concluding Remark

Numerics like those contained herein can be used to design efficient algorithms for Gaussian quadrature associated with ordered orthogonal Laurent polynomial sequences.

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FIGURE 1. Weight function w(x)=1 on [1,2] graph and corresponding plots of minimal universal compass readings as a function of rank n and trailing power p.

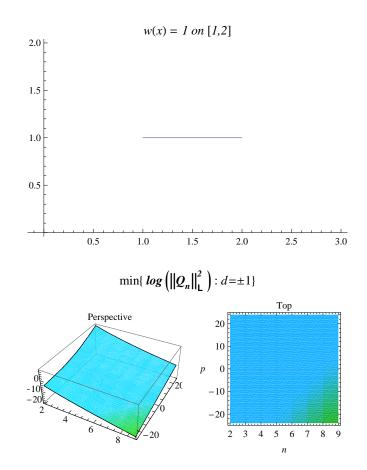
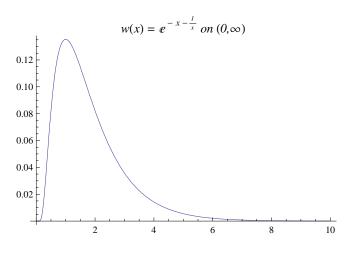


FIGURE 2. Weight function $w(x)=e^{-x-1/x}$ on $(0,\infty)$ along with corresponding table and plots of minimal universal compass readings as a function of rank n and trailing power p.



n	đ	p	$\left\ Q_{n}\right\ _{\mathcal{L}}^{2}$	log $\left(\left\ \mathcal{Q}_{n}\right\ _{\mathcal{L}}^{2}\right)$
2	1	- 2	0.08079612518	-1.0926094666
2	-1	1	0.08079612518	-1.0926094666
3	1	- 3	0.03487232568	-1.4575190880
3	-1	2	0.03487232568	-1.4575190880
4	1	-4	0.01810285907	-1.7422528295
4	-1	3	0.01810285907	-1.7422528295
5	1	- 5	0.01048504769	-1.9794295897
5	-1	4	0.01048504769	-1.9794295897
6	1	- 6	0.006536793386	-2.1846352419
6	-1	5	0.006536793386	-2.1846352419
7	1	-7	0.004298798555	-2.3666529058
7	-1	6	0.004298798555	-2.3666529058
8	1	- 8	0.002944637121	-2.5309682174
8	-1	7	0.002944637121	-2.5309682174
9	1	- 9	0.002083248156	-2.6812589940
9	-1	8	0.002083248156	-2.6812589940

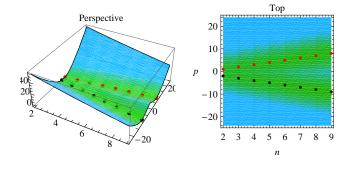
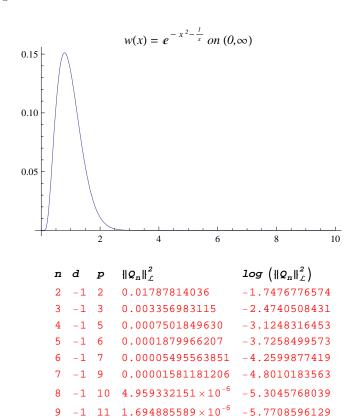


FIGURE 3. Weight function $w(x) = e^{-x^2 - 1/x}$ on $(0, \infty)$ along with corresponding table and plots of minimal universal compass readings.



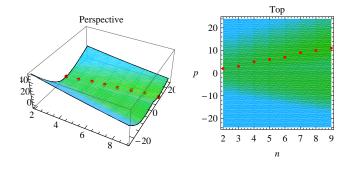
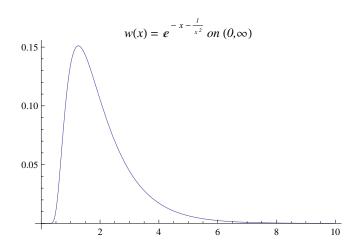


FIGURE 4. Weight function $w(x) = e^{-x-1/x^2}$ on $(0, \infty)$ along with corresponding table and plots of minimal universal compass readings.



n	d	p	$\left\ Q_{n}\right\ _{\mathcal{L}}^{2}$	$log\left(\left\ \mathcal{Q}_{n} ight\ _{\mathcal{L}}^{2} ight)$
2	1	- 3	0.01787814036	-1.7476776574
3	1	-4	0.003356983115	-2.4740508431
4	1	-6	0.0007501849630	-3.1248316453
5	1	-7	0.0001879966207	-3.7258499573
6	1	- 8	0.00005495563851	-4.2599877419
7	1	-10	0.00001581181206	-4.8010183563
8	1	-11	$4.959332151\times 10^{-6}$	-5.3045768039
9	1	-12	$1.694885589 \times 10^{-6}$	-5.7708596129

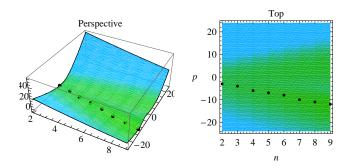
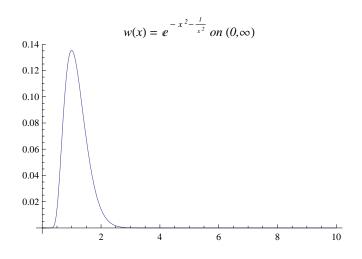


FIGURE 5. Weight function $w(x)=e^{-x^2-1/x^2}$ on $(0,\infty)$ along with corresponding table and plots of minimal universal compass readings.



n	d	p	$\left\ \mathcal{Q}_{n} \right\ _{\mathcal{L}}^{2}$	$\log\left(\left\ \mathcal{Q}_{n}^{} ight\ _{\mathcal{L}}^{2} ight)$
2	1	- 2	0.01120102415	-1.9507422664
2	-1	1	0.01120102415	-1.9507422664
3	1	- 3	0.001727464284	-2.7625909230
3	-1	2	0.001727464284	-2.7625909230
4	1	- 4	0.0003442296230	-3.4631517588
4	-1	3	0.0003442296230	-3.4631517588
5	1	- 5	0.00008086014809	-4.0922654676
5	-1	4	0.00008086014809	-4.0922654676
6	1	- 7	0.00002094601062	-4.6788986806
6	-1	6	0.00002094601062	-4.6788986806
7	1	- 8	$5.769581136 \times 10^{-6}$	-5.2388557149
7	-1	7	$5.769581136 \times 10^{-6}$	-5.2388557149
8	1	- 9	$1.716340692\times 10^{-6}$	-5.7653965010
8	-1	8	$1.716340692 \times 10^{-6}$	-5.7653965010
9	1	-10	$5.439211462 \times 10^{-7}$	-6.2644640567
9	-1	9	$5.439211462 \times 10^{-7}$	-6.2644640567

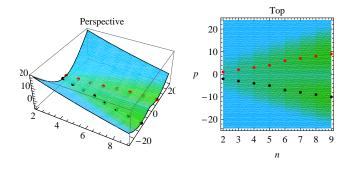
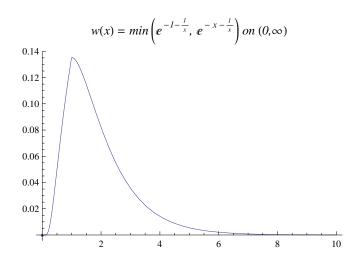


FIGURE 6. Weight function $w(x)=\min\left(e^{-1-1/x},e^{-x-1/x}\right)$ on $(0,\infty)$ along with corresponding table and plots of minimal universal compass readings.



n	đ	p	$\left\ \mathcal{Q}_{n} \right\ _{\mathcal{L}}^{2}$	log $\left(\left\ \mathcal{Q}_{n}\right\ _{\mathcal{L}}^{2}\right)$
2	1	- 2	0.06304693809	-1.2003360004
3	1	- 3	0.02743883885	-1.5616342709
4	-1	3	0.01395887495	-1.8551495833
5	-1	4	0.007760510589	-2.1101097042
6	-1	5	0.004695195765	-2.3283462952
7	-1	6	0.003020905036	-2.5198629268
8	-1	7	0.002035655433	-2.6912957314
9	-1	8	0.001421546080	-2.8472390580

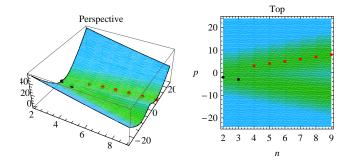
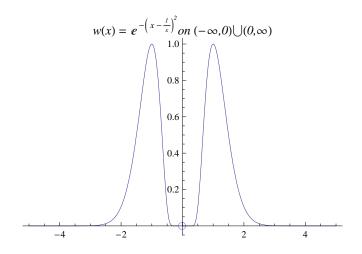


FIGURE 7. Weight function $w(x) = e^{-(x-1/x)^2}$ on \mathbb{R}^* given by the doubling transformation in the classical Hermite case, followed by the corresponding table and plots of minimal universal compass readings as a function of rank n and trailing power p.



n	đ	p	$\left\ \mathcal{Q}_{n} \right\ _{\mathcal{L}}^{2}$	log $\left(\left\ \mathcal{Q}_{n}\right\ _{\mathcal{L}}^{2}\right)$
2	1	-1	1.772453851	0.2485749363
2	1	- 2	1.772453851	0.2485749363
2	-1	1	1.772453851	0.2485749363
2	-1	0	1.772453851	0.2485749363
3	1	- 3	0.5453704157	-0.2633084246
3	-1	2	0.5453704157	-0.2633084246
4	1	-4	0.5453704157	-0.2633084246
4	-1	3	0.5453704157	-0.2633084246
5	1	- 5	0.2465671264	-0.6080648263
5	-1	4	0.2465671264	-0.6080648263
6	1	-6	0.2465671264	-0.6080648263
6	-1	5	0.2465671264	-0.6080648263
7	1	-7	0.1327717941	-0.8768941761
7	-1	6	0.1327717941	-0.8768941761
8	1	- 8	0.1327717941	-0.8768941761
8	-1	7	0.1327717941	-0.8768941761
9	1	- 9	0.07926184182	-1.1009358401
9	-1	8	0.07926184182	-1.1009358401

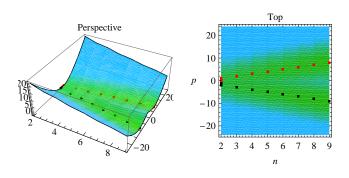
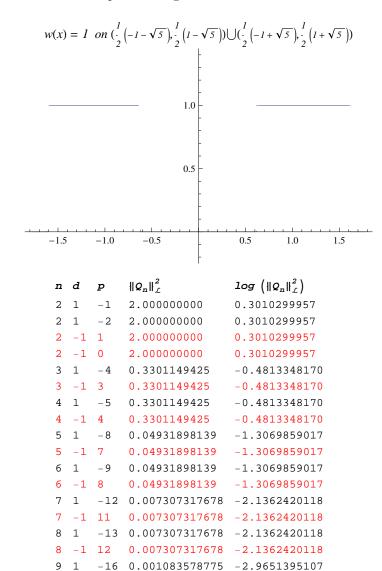
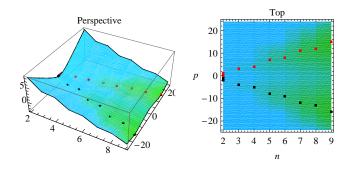


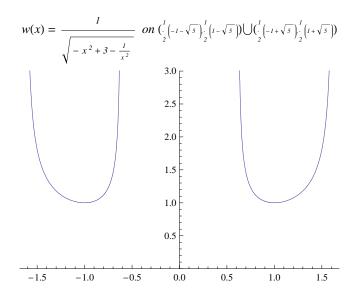
FIGURE 8. Legendre-type weight function given by the doubling transformation, followed by corresponding table and plots of minimal universal compass readings.





0.001083578775 -2.9651395107

FIGURE 9. Tchebycheff-type weight function given by the doubling transformation, followed by corresponding table and plots of minimal universal compass readings.



n	đ	p	$\left\ \mathcal{Q}_{n} \right\ _{\mathcal{L}}^{2}$	$log\left(\left\ \mathcal{Q}_{n} ight\ _{\mathcal{L}}^{2} ight)$
2	1	-1	3.141592654	0.4971498727
2	1	- 2	3.141592654	0.4971498727
2	-1	1	3.141592654	0.4971498727
2	-1	0	3.141592654	0.4971498727
3	1	- 5	0.4933241376	-0.3068676347
3	-1	4	0.4933241376	-0.3068676347
4	1	-6	0.4933241376	-0.3068676347
4	-1	5	0.4933241376	-0.3068676347
5	1	- 9	0.07379325022	-1.1319833608
5	-1	8	0.07379325022	-1.1319833608
6	1	-10	0.07379325022	-1.1319833608
6	-1	9	0.07379325022	-1.1319833608
7	1	-12	0.01063460561	-1.9732786115
7	-1	11	0.01063460561	-1.9732786115
8	1	-13	0.01063460561	-1.9732786115
8	-1	12	0.01063460561	-1.9732786115
9	1	-16	0.001545863844	-2.8108287602
9	-1	15	0.001545863844	-2.8108287602

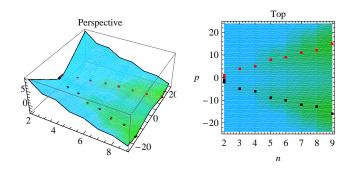
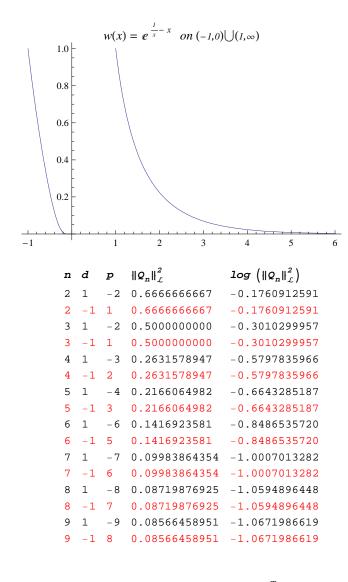


FIGURE 10. Laguerre-type weight function given by the doubling transformation, followed by corresponding table and plots of minimal universal compass readings.



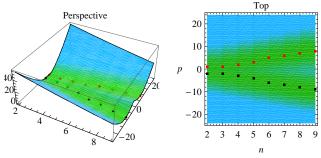
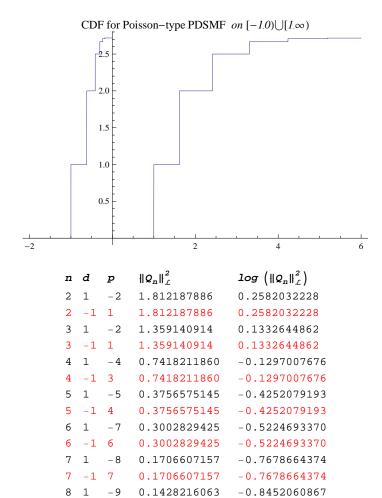
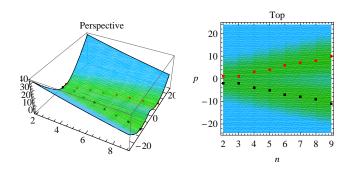


FIGURE 11. Poisson-type cumulative distribution function (CDF) given by the doubling transformation, followed by corresponding table and plots of minimal universal compass readings as a function of rank n and trailing power p.





0.1428216063

-11 0.09855119037

-1 10

-0.8452060867

-1.0063381256

0.09855119037 -1.0063381256