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Error Bounds for Gauss-Lobatto Quadrature Formula with Multiple End Points with Chebyshev Weight Function of the Third and the Fourth Kind

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Abstract. For analytic functions the remainder terms of quadrature formulae can be represented as a contour integral with a complex kernel. We study the kernel, on elliptic contours with foci at the points ∓ 1, for Gauss-Lobatto quadrature formula with multiple end points with Chebyshev weight function of the third and the fourth kind. Starting from the explicit expression of the corresponding kernel, derived by Gautschi and Li, we determine the locations on the ellipses where maximum modulus of the kernel is attained. The obtained values confirm the corresponding conjectured values given by Gautschi and Li in paper [The remainder term for analytic functions of Gauss-Radau and Gauss-Lobatto quadrature rules with multiple end points, Journal of Computational and Applied Mathematics 33 (1990) 315-329.]

1. Introduction

In this paper, we analyze the remainder term of Gauss-Lobatto quadrature rule with the end points ∓ 1 of multiplicity r,

$$\int_{-1}^{1} f(t)\omega(t)\,dt = \sum_{\rho=0}^{r-1} \kappa_\rho{}^L f^{(\rho)}(-1) + \sum_{\rho=0}^{r-1} \mu_\rho{}^L f^{(\rho)}(1) + \sum_{\nu=1}^{n} \lambda_\nu{}^L f(\tau_\nu{}^L) + R_{n,r}^L(f), \tag{1}$$

where $\tau_\nu{}^L$ are zeros of $\pi_n(\cdot;\omega^L)$, orthogonal polynomial on $[-1,1]$, with respect to the weight function

$$\omega^L(t) = (t^2-1)^r\omega(t).$$

Also, $R_{n,r}^L(f) = 0$ for all $f \in \mathbb{P}_{2n+2r-1}$ (the set of polynomial of degree $\le 2n+2r-1$).

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Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1,1]$ and let $\mathcal{D} = \mathrm{int}\Gamma$ be its interior. If the integrand f is analytic in a domain $\mathcal{D}$ containing $[-1,1]$, then the remainder term $R^L_{n,r}(f)$ admits the contour integral representation

$$R^L_{n,r}(f) = \frac{1}{2\pi i}\oint_\Gamma K^L_{n,r}(z;\omega)f(z)dz. \tag{2}$$

The *kernel* is given by

$$K^L_{n,r}(z;\omega) \equiv K_{n,r}(z,\omega) = \frac{\varrho^L_{n,r}(z;\omega)}{(z^2-1)^r\pi_n(z;\omega^L)}, \quad z \notin [-1,1],$$

where, if we denote $(z^2-1)^r\pi_n(z;\omega^L) = \omega_{n,r}(z;\omega)$,

$$\varrho^L_{n,r}(z;\omega) \equiv \varrho_{n,r}(z,\omega) = \int_{-1}^{1}\frac{\omega_{n,r}(z;\omega)}{z-t}\,\omega(t)dt.$$

The integral representation (2) leads to the error bound

$$|R^L_{n,r}(f)| \le \frac{\ell(\Gamma)}{2\pi}\left(\max_{z\in\Gamma}|K_{n,r}(z;\omega)|\right)\left(\max_{z\in\Gamma}|f(z)|\right),$$

where $\ell(\Gamma)$ is the length of the contour Γ.

In this paper we take $\Gamma = \mathcal{E}_\rho$, where the ellipse $\mathcal{E}_\rho$ is given by

$$\mathcal{E}_\rho = \left\{z \in \mathbb{C} \mid z = \frac{1}{2}\left(u+u^{-1}\right),\ 0 \le \theta \le 2\pi\right\}, \quad u = \rho\, e^{i\theta}. \tag{3}$$

The upper bound of $|R^L_{n,r}(f)|$ reduces to

$$|R^L_{n,r}(f)| \le \frac{\ell(\mathcal{E}_\rho)}{2\pi}\left(\max_{z\in\mathcal{E}_\rho}|K_{n,r}(z;\omega)|\right)\left(\max_{z\in\mathcal{E}_\rho}|f(z)|\right).$$

Furthermore, we take $r = 2$, meaning we are dealing with endpoints of multiplicity 2.
The goal is to determine the points where the kernel attains its maximum modulus along the contour of integration.

When $\rho \longrightarrow 1$, the ellipse (1.3) shrinks to the interval $[-1,1]$, while with increasing ρ it becomes more and more circle-like. The advantage of elliptical contours over circular ones is that such a choice requires the analyticity of f in a smaller region of the complex plane, especially when ρ is near 1.

In [2] Gautschi considered Gauss-Radau and Gauss-Lobatto quadrature rules with multiple end points with respect to the four Chebyshev weight functions

$$\omega_1(t) = \frac{1}{\sqrt{1-t^2}}, \quad \omega_2(t) = \sqrt{1-t^2}, \quad \omega_3(t) = \sqrt{\frac{1+t}{1-t}}, \quad \omega_4(t) = \sqrt{\frac{1-t}{1+t}},$$

and derived explicit expressions of the corresponding kernels $K(z;\omega_j)$, $j = 1,2,3,4$, in terms of the variable $u = \rho e^{i\theta}$.

For Gauss-Radau quadratures with a fixed node at -1, Gautschi in [1] proved that the corresponding kernel for Chebyshev weight functions $\omega = \omega_1$ and $\omega = \omega_4$ attains its maximum modulus on $\mathcal{E}_\rho$ on the negative real axis. Recently, Pejčev and Spalević [4] proved and confirmed the empirical results from [1] in the case $\omega = \omega_3$. Milovanović, Spalević and Pranić in [3] also proved and confirmed the empirical results from [1] in the case $\omega = \omega_2$.
For Gauss-Lobatto quadratures with multiple end points with Chebyshev weight function of the first kind it is proved that $|K_{n,2}(z;\omega_1)|$ attains its maximum on $\mathcal{E}_\rho$ on the real axis (cf. [2, Theorem 4.1]). For ω_2 numerical and asymptotic results were presented.

For ω_3 and ω_4 Gautschi and Li in [2] presented the *statement* based on numerical and asymptotic results. In this paper we prove the existence of the fixed value from the *statement* analytically and give strong numerical evidence.

2. Maximum of the Modulus of the Kernel for Gauss-Lobatto Quadrature with Multiple End Points

For $\omega = \omega_3$ in the Gauss-Lobatto quadrature formula (1), there is a suggestion (cf. Gautschi and Li [2, pg. 328]) that the maximum is always attained on the positive real axis.
Gautschi and Li [1, Eqs. (2.17) and (2.18)] derived the explicit representations of the kernels on $\mathcal{E}_\rho$,

$$K_{n,2}(z;\omega_3) = \frac{2\pi}{u^{n+4}}\frac{u+1}{u-1}$$
$$\times\frac{u^3+\alpha(u^2-u)-\beta}{\beta[u^{n+4}-u^{-(n+4)}]+\alpha[u^{n+3}-u^{-(n+3)}-(u^{n+2}-u^{-(n+2)})]-[u^{n+1}-u^{-(n+1)}]},$$

and $K_{n,2}(z;\omega_4) = -K_{n,2}(-z;\omega_3)$,
where $\alpha = \dfrac{n+1}{n+3}$, $\beta = \dfrac{(n+1)(n+2)}{(n+3)(n+4)}$, $z = (u+u^{-1})/2$ and $u = \rho e^{i\theta}$.
We can determine the modulus of the kernel on $\mathcal{E}_\rho$. We are also interested in the modulus of the kernel at $\theta = 0$ because the corresponding Gautschi and Li's *statement* claims that the modulus of the kernel attains its maximum at $\theta = 0$ for all $\rho > 1$. First, we consider $K_{n,2}(z;\omega_3)$, and later, because of the simplicity reasons and the symmetry, analogue results are presented for $K_{n,2}(z;\omega_4)$.
By introducing some substitutions, we can easily express the modulus of the kernel in the following form

$$|K_{n,2}(z;\omega_3)| = \sqrt{\frac{4\pi^2}{\rho^{2n+8}}\frac{ac}{b\delta}},$$

where

$$\begin{aligned}
a &= |u+1|^2 = \rho^2 + 2\cos\theta\cdot\rho + 1,\\
b &= |u-1|^2 = \rho^2 - 2\cos\theta\cdot\rho + 1,\\
c &= |u^3+\alpha(u^2-u)-\beta|^2\\
&= \rho^6 + (2\alpha\cos\tfrac{\theta}{2})\cdot\rho^5 + (\alpha^2 - 2\alpha\cos\theta)\cdot\rho^4\\
&+ (-2\alpha^2\cos\tfrac{\theta}{2} - 2\beta\cos\tfrac{3\theta}{2})\cdot\rho^3\\
&+ (\alpha^2 - 2\alpha\beta\cos\theta)\cdot\rho^2 + (2\alpha\beta\cos\tfrac{\theta}{2})\cdot\rho + \beta^2\\
\delta &= \left|\beta[u^{n+4}-u^{-(n+4)}]+\alpha[u^{n+3}-u^{-(n+3)}-(u^{n+2}-u^{-(n+2)})]-[u^{n+1}-u^{-(n+1)}]\right|^2\\
&= \frac{d}{\rho^{2n+8}},
\end{aligned}$$

i. e.

$$
\begin{aligned}
d &= \delta \cdot \rho^{2n+8} = |\beta[u^{n+4} - u^{-(n+4)}] \\
&+ \alpha[u^{n+3} - u^{-(n+3)} - (u^{n+2} - u^{-(n+2)})] - [u^{n+1} - u^{-(n+1)}]|^2 \cdot \rho^{2n+8} \\
&= \beta^2 \cdot \rho^{4n+16} + (2\alpha\beta\cos\theta) \cdot \rho^{4n+15} + (\alpha^2 - 2\alpha\beta\cos 2\theta) \cdot \rho^{4n+14} \\
&+ (-2\beta\cos 3\theta - 2\alpha^2\cos\theta) \cdot \rho^{4n+13} + (\alpha^2 - 2\alpha\cos 2\theta) \cdot \rho^{4n+12} \\
&+ (2\alpha\cos\theta) \cdot \rho^{4n+11} + \rho^{4n+10} + (2\beta\cos(2n+5)\theta) \cdot \rho^{2n+11} \\
&+ (2\alpha\beta\cos(2n+6)\theta + 2\alpha\cos(2n+4)\theta) \cdot \rho^{2n+10} \\
&+ (2\alpha^2\cos(2n+5)\theta - 2\alpha\beta\cos(2n+7)\theta - 2\alpha\cos(2n+3)\theta) \cdot \rho^{2n+9} \\
&+ (-2\beta^2\cos(2n+8)\theta - 2\cos(2n+2)\theta \\
&- 2\alpha^2\cos(2n+6)\theta - 2\alpha^2\cos(2n+4)\theta) \cdot \rho^{2n+8} \\
&+ (-2\alpha\beta\cos(2n+7)\theta - 2\alpha\cos(2n+3)\theta + 2\alpha^2\cos(2n+5)\theta) \cdot \rho^{2n+7} \\
&+ (2\alpha\cos(2n+4)\theta + 2\alpha\beta\cos(2n+6)\theta) \cdot \rho^{2n+6} + (2\beta\cos(2n+5)\theta) \cdot \rho^{2n+5} \\
&+ \rho^6 + (2\alpha\cos\theta) \cdot \rho^5 + (\alpha^2 - 2\alpha\cos 2\theta) \cdot \rho^4 + (-2\alpha^2\cos\theta - 2\beta\cos 3\theta) \cdot \rho^3 \\
&+ (\alpha^2 - 2\alpha\beta\cos 2\theta) \cdot \rho^2 + (2\alpha\beta\cos\theta) \cdot \rho + \beta^2.
\end{aligned}
$$

In order to express $d(\rho)$ as a polynomial function in ρ, the term δ was multiplied by ρ^{2n+8}, which reduces the expression for the square of the modulus of the kernel to

$$\left|K_{n,2}(z;\omega_3)\right|^2 = 4\pi^2 \frac{ac}{bd}.$$

By letting A, B, C, D denote the values of a, b, c, d for $\theta = 0$, the square of the modulus of the kernel for $\theta = 0$ can be expressed as

$$|K_{n,2}(z;\omega_3)|^2 = 4\pi^2 \frac{AC}{BD}.$$

Our aim is to show that this is the maximum value of the modulus for all $\rho > 1$ and $\theta \in [0, 2\pi]$.

The following substitutions are appropriate:

$$\begin{aligned}
A &= \rho^2 + 2\rho + 1, \\
B &= \rho^2 - 2\rho + 1, \\
C &= \rho^6 + 2\alpha \cdot \rho^5 + (\alpha^2 - 2\alpha) \cdot \rho^4 \\
&+ (-2\alpha^2 - 2\beta) \cdot \rho^3 + (\alpha^2 - 2\alpha\beta) \cdot \rho^2 + 2\alpha\beta \cdot \rho + \beta^2, \\
D &= \beta^2 \cdot \rho^{4n+16} + (2\alpha\beta) \cdot \rho^{4n+15} + (\alpha^2 - 2\alpha\beta) \cdot \rho^{4n+14} + (-2\beta - 2\alpha^2) \cdot \rho^{4n+13} \\
&+ (\alpha^2 - 2\alpha) \cdot \rho^{4n+12} + (2\alpha) \cdot \rho^{4n+11} + \rho^{4n+10} + (2\beta) \cdot \rho^{2n+11} \\
&+ (2\alpha\beta + 2\alpha) \cdot \rho^{2n+10} + (2\alpha^2 - 2\alpha\beta - 2\alpha) \cdot \rho^{2n+9} + (-2\beta^2 - 2 - 4\alpha^2) \cdot \rho^{2n+8} \\
&+ (-2\alpha\beta - 2\alpha + 2\alpha^2) \cdot \rho^{2n+7} + (2\alpha + 2\alpha\beta) \cdot \rho^{2n+6} + (2\beta) \cdot \rho^{2n+5} \\
&+ \rho^6 + (2\alpha) \cdot \rho^5 + (\alpha^2 - 2\alpha) \cdot \rho^4 + (-2\alpha^2 - 2\beta) \cdot \rho^3 \\
&+ (\alpha^2 - 2\alpha\beta) \cdot \rho^2 + (2\alpha\beta) \cdot \rho + \beta^2.
\end{aligned}$$

3. The Main Results

According to Gautschi and Li's *statement*, the maximum modulus of the kernel is attended on the real axis for all $\rho > \rho^*(n) = 1$. We formulate the following theorem, which states the existence of that value, and provides an analytical proof. Whereas the suggestion that the result holds for all ρ from the interval $(1, \infty)$, some cases are confirmed through a detailed numerical study.

Theorem 3.1. *For the Gauss-Lobatto quadrature formula with multiple end points* ∓ 1 $(r = 2)$ *with the Chebyshev weight function of the third kind, there exist a value* $\rho^*(n)$ *such that the modulus of the kernel* $\left|K_{n,2}(z;\omega_3)\right|$ *attains its maximum value on the positive real semi axis* $(\theta = 0)$ *for each* $\rho > \rho^*(n)$*, i.e.*

$$\max_{z\in\mathcal{E}_\rho} \left|K_{n,2}(z;\omega_3)\right| = \left|K_{n,2}\left(\frac{1}{2}(\rho + \rho^{-1}), \omega_3\right)\right|$$

for each $\rho > \rho^*(n)$.

Proof. Referring to the previously introduced notation, we have to show that

$$\frac{ac}{bd} \le \frac{AC}{BD}.$$

for each ρ greater than some $\rho^*(n)$. We can simplify this inequality by denoting A_1, B_1, C_1, D_1 the differences

$a - A$, $b - B$, $c - C$ and $d - D$ respectively, i.e.

$$\begin{aligned}
A_1 &= 4 \cdot (\sin^2 \tfrac{\theta}{2}) \cdot \rho, \\
B_1 &= -4 \cdot (\sin^2 \tfrac{\theta}{2}) \cdot \rho, \\
C_1 &= 4 \cdot [(-\alpha \sin^2 \tfrac{\theta}{2}) \cdot \rho^5 + (\alpha \sin^2 \theta) \cdot \rho^4 + (\beta \sin^2 \tfrac{3\theta}{2} + \alpha^2 (\sin^2 \tfrac{\theta}{2})) \cdot \rho^3 \\
&+ (\alpha\beta \sin^2 \theta) \cdot \rho^2 + (-\alpha\beta \sin^2 \tfrac{\theta}{2}) \cdot \rho], \\
D_1 &= 4 \cdot [(-\alpha\beta \sin^2 \frac{\theta}{2}) \cdot \rho^{4n+15} + (\alpha\beta \sin^2 \theta) \cdot \rho^{4n+14} \\
&+ (\beta \sin^2 \tfrac{3\theta}{2} + \alpha^2 \sin^2 \tfrac{\theta}{2}) \cdot \rho^{4n+13} + (\alpha \sin^2 \theta) \cdot \rho^{4n+12} + (-\alpha \sin^2 \tfrac{\theta}{2}) \cdot \rho^{4n+11} \\
&+ (-\beta \sin^2 \tfrac{(2n+5)\theta}{2}) \cdot \rho^{2n+11} + (-\alpha\beta \sin^2 \tfrac{(2n+6)\theta}{2} - \alpha \sin^2 \tfrac{(2n+4)\theta}{2}) \cdot \rho^{2n+10} \\
&+ (-\alpha^2 \sin^2 \tfrac{(2n+5)\theta}{2} + \alpha\beta \sin^2 \tfrac{(2n+7)\theta}{2} + \alpha \sin^2 \tfrac{(2n+3)\theta}{2}) \cdot \rho^{2n+9} \\
&+ (\beta^2 \sin^2 \tfrac{(2n+8)\theta}{2} + \sin^2 \tfrac{(2n+2)\theta}{2} + \alpha^2 \sin^2 \tfrac{(2n+6)\theta}{2} + \alpha^2 \sin^2 \tfrac{(2n+4)\theta}{2}) \cdot \rho^{2n+8} \\
&+ (\alpha\beta \sin^2 \tfrac{(2n+7)\theta}{2} + \alpha \sin^2 \tfrac{(2n+3)\theta}{2} - \alpha^2 \sin^2 \tfrac{(2n+5)\theta}{2}) \cdot \rho^{2n+7} \\
&+ (-\alpha \sin^2 \tfrac{(2n+4)\theta}{2} - \alpha\beta \sin^2 \tfrac{(2n+6)\theta}{2}) \cdot \rho^{2n+6} + (-\beta \sin^2 \tfrac{(2n+5)\theta}{2}) \cdot \rho^{2n+5} \\
&+ (-\alpha \sin^2 \tfrac{\theta}{2}) \cdot \rho^5 + (\alpha \sin^2 \theta) \cdot \rho^4 + (\alpha^2 \sin^2 \tfrac{\theta}{2} + \beta \sin^2 \tfrac{3\theta}{2}) \cdot \rho^3 \\
&+ (\alpha\beta \sin^2 \theta) \cdot \rho^2 + (-\alpha\beta \sin^2 \tfrac{\theta}{2}) \cdot \rho].
\end{aligned}$$

The previous inequality can be written as:

$$I = I(\rho) = [CD(A_1 B - AB_1) + C_1 BD(A + A_1) - AC(B + B_1)D_1] \leq 0, \tag{4}$$

for each $\rho > \rho^*(n)$.

We can easily see that I is a polynomial in ρ of degree equal to $4n + 25$, whose coefficients depend only on θ, i.e.

$$I = I(\rho) = \sum_{i=0}^{4n+25} a_i(\theta)\rho^i. \tag{5}$$

In order to show the existence of number $\rho^*(n)$, we use the well– known fact that, starting from some value of ρ, the sign of polynomial $I(\rho) = \rho^{4n+25}(a_{4n+25} + \frac{a_{4n+24}}{\rho} + \frac{a_{4n+23}}{\rho^2} + \ldots + \frac{a_0}{\rho^{4n+25}})$ coincides with the sign of its leading coefficient. So, it is enough to analyze leading coefficient a_{4n+25} and to show its negativity.

Decomposing $I(\rho)$ into sum: $I(\rho) = x(\rho) + y(\rho) - z(\rho)$, and considering the highest order coefficients of $x(\rho), y(\rho)$ and $z(\rho)$ we get respectively: $\beta^2(-8 \sin^2 \frac{\theta}{2})$, $-4\alpha\beta^2 \sin^2 \frac{\theta}{2}$ and $(-4\alpha\beta \sin^2 \frac{\theta}{2})$. Putting them together give

$a_{4n+25} = -8\beta^2 \sin^2 \frac{\theta}{2} - 4\alpha\beta^2 \sin^2 \frac{\theta}{2} + 4\alpha\beta \sin^2 \frac{\theta}{2} = -4\beta \sin^2 \frac{\theta}{2}(2\beta + \alpha\beta - \alpha)$,

where $\alpha = \dfrac{n+1}{n+3}$ and $\beta = \dfrac{(n+1)(n+2)}{(n+3)(n+4)} = \alpha \cdot \dfrac{n+2}{n+4}$. Therefore,

$$a_{4n+25} < 0 \quad \textbf{iff} \quad 2\beta + \alpha\beta - \alpha > 0 \quad \textbf{iff} \quad 2\frac{n+2}{n+4} + \frac{(n+1)(n+2)}{(n+3)(n+4)} - 1 > 0.$$

The previous inequality reduces to $n^2 + 3n + 1 > 0$ which is true for each $n > 0$, so negativity of the a_{4n+25} is obvious. □

Similar result holds for $K_{n,2}(z;\omega_4)$ $(= -K_{n,2}(-z;\omega_3))$.

Theorem 3.2. *For the Gauss-Lobatto quadrature formula with multiple end points* ± 1 $(r = 2)$ *with the Chebyshev weight function of the fourth kind, there exist a value* $\rho^*(n)$ *such that the modulus of the kernel* $\left|K_{n,2}(z;\omega_4)\right|$ *attains its maximum value on the negative real semi axis* $(\theta = \pi)$ *for each* $\rho > \rho^*(n)$, *i.e.*

$$\max_{z\in\mathcal{E}_\rho} \left|K_{n,2}(z;\omega_4)\right| = \left|K_{n,2}\left(-\frac{1}{2}(\rho+\rho^{-1}),\omega_4\right)\right|$$

for each $\rho > \rho^*(n)$.

3.1. Gautschi and Li's statement

According to *statement*, the maximum is attended at $\theta = 0$ for all $\rho > 1$. In order to ensure the non-positivity of the polynomial $I(\rho)$ given by (5) for each $\rho > 1$, we can write initial polynomial as a polynomial in $\rho - 1$, and show the non-positivity of its new coefficients. We have

$I(\rho) = \sum_{i=0}^{4n+25} b_i(\theta)(\rho-1)^i$ for all $\rho > 1$.

Numerical computations show that all functions $b_i(\theta),\ i = 0,1,\dots,4n+25$ are strictly under the x-axis for all θ from the interval $[0,2\pi]$. In general, the non-positivity of the coefficients $b_i(\theta)$ is not necessary condition for non-positivity of a polynomial for each $\rho > 1$, but in this case, it is obviously a sufficient condition. Explicit formulae for coefficients $b_i(\theta),\ i = 0,1,\dots,4n+25$, can be given in the terms of the coefficients $a_i(\theta)$ by using the binomial formula, but in `MATLAB` implementation it is more practical to use Horner scheme. The new coefficients $b_0, b_1, \dots, b_{4n+25}$ are complicated trigonometric functions of θ, inappropriate for analytical considerations.

The method has been tested for all values of n from 1 to 100 and it gives the optimal results in all the cases. Some of the cases are displayed in Figs. 1 and 2.

Figure 1: The functions $b_0(\theta), \ldots, b_{33}(\theta)$, in the case $n = 2$ (left) and the functions $b_0(\theta), \ldots, b_{45}(\theta)$, in the case $n = 5$ (right).

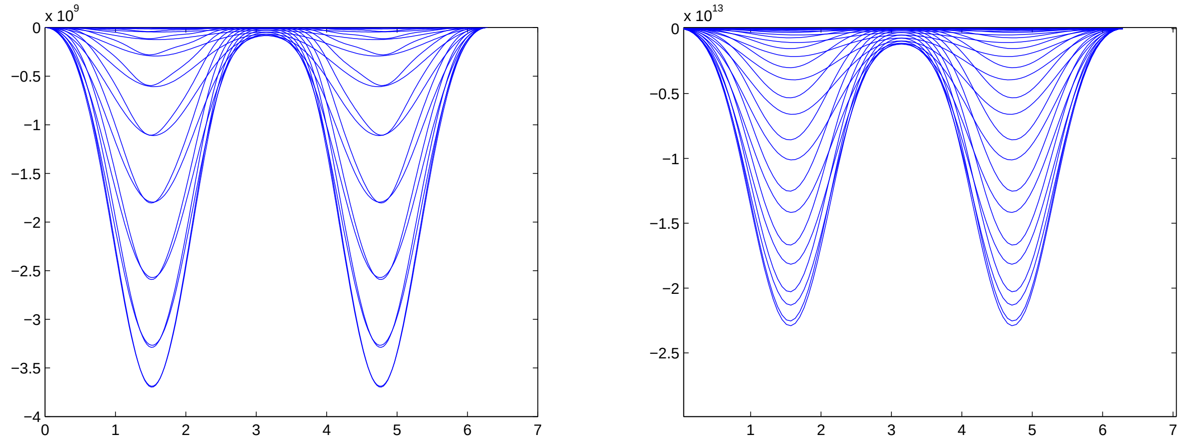
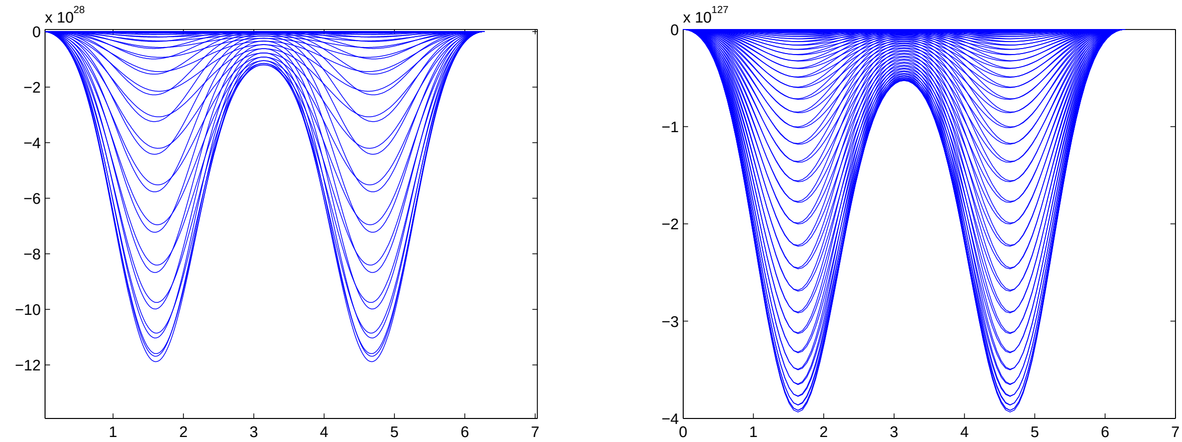


Figure 2: The functions $b_0(\theta), \ldots, b_{97}(\theta)$, in the case $n = 18$ (left) and the functions $b_0(\theta), \ldots, b_{425}(\theta)$, in the case $n = 100$ (right.)



Numerical results also show that the graphs of polynomials $I(n, \rho, \theta)$ are strictly non-positive for each $n \in \mathbb{N}$, $\rho > 1$ and $\theta \in [0, 2\pi]$. Some of these cases are displayed in Figs. 3 and 4.

Figure 3: The functions $I(\theta)$ in the case $n = 1$, $\rho = 1.0001$ (left) and in the case $n = 13$, $\rho = 1.0001$ (right).

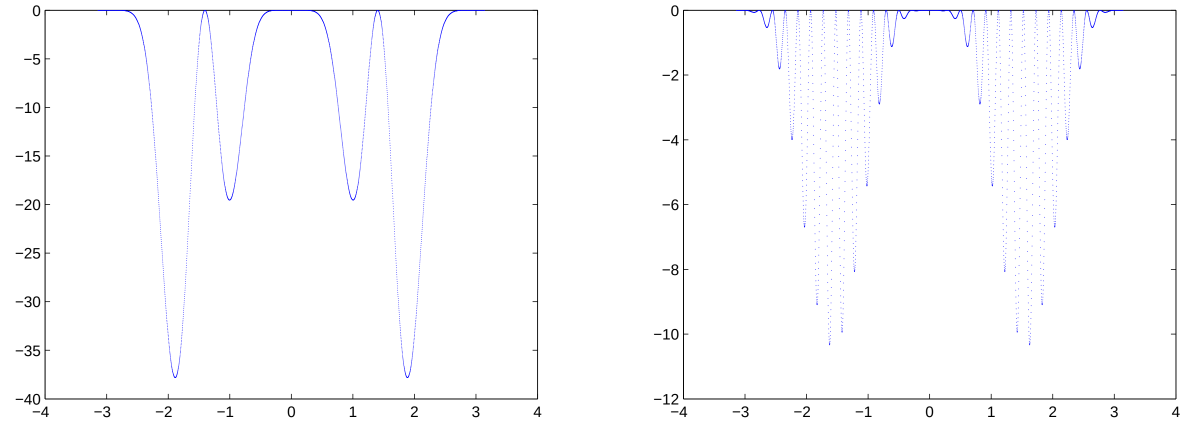
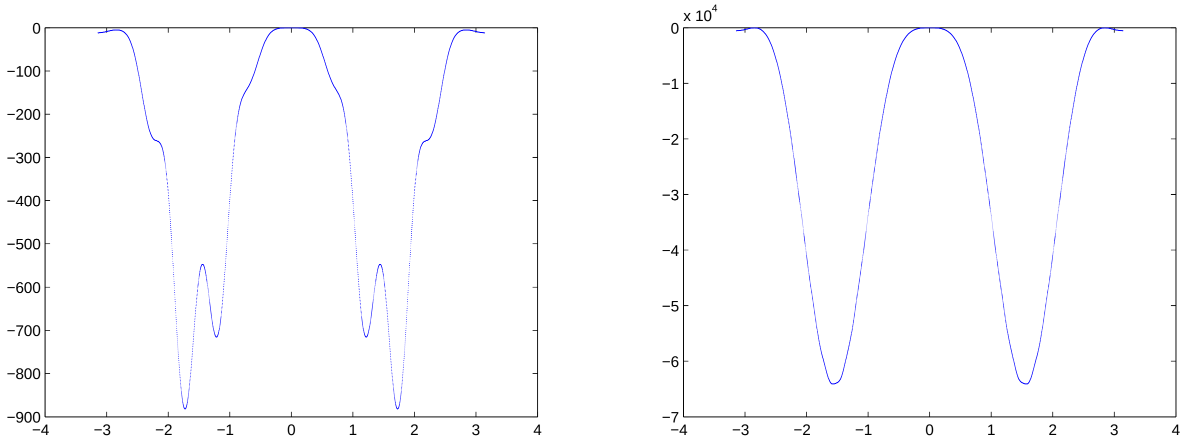


Figure 4: The functions $I(\theta)$ in the case $n = 3$, $\rho = 1.2$ (left) and in the case $n = 15$, $\rho = 1.2$ (right).



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