A Lagrange series approach to the spectrum of the Kite

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A LAGRANGE SERIES APPROACH TO THE SPECTRUM OF THE KITE GRAPH∗

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Abstract. A Lagrange series around adjustable expansion points to compute the eigenvalues of graphs, whose characteristic polynomial is analytically known, is presented. The computations for the kite graph $P_nK_m$, whose largest eigenvalue was studied by Stevanović and Hansen [D. Stevanović and P. Hansen. The minimum spectral radius of graphs with a given clique number. Electronic Journal of Linear Algebra, 17:110–117, 2008.], are illustrated. It is found that the first term in the Lagrange series already leads to a better approximation than previously published bounds.

Key words. Spectrum of a graph, Lagrange series, Characteristic polynomial.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Let $A_G$ denote the $N \times N$ adjacency matrix of the graph $G$ on $N$ nodes. If we denote the inverse function $\lambda = c_{A_G}^{-1}(w)$ of the characteristic polynomial $w = c_{A_G}(\lambda) = \det(AG - \lambda I)$, then an eigenvalue of $A_G$ satisfies $\lambda_k = c_{A_G}^{-1}(0)$, where the eigenvalues are ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$. The Lagrange series of $c_{A_G}(\lambda)$ returns the series expansion of $c_{A_G}^{-1}(w)$ around an expansion point $w_0 = c_{A_G}(\lambda_0)$. The coefficients of the Lagrange series of a function are more complicated to compute analytically than the coefficients of its Taylor series. However, we have shown, by introducing our characteristic coefficients [8] (briefly summarized in Section 3 below) that all coefficients of the Lagrange series around $w_0$ can be computed from the Taylor series coefficients around an expansion point $\lambda_0$. The knowledge of a good expansion point $w_0 = c_{A_G}(\lambda_0)$ is crucial for the converge of a Lagrange series [12], but is, in general, not easy to determine, unless a good grasp of the zero (here the eigenvalue $\lambda_k$) is known. The main contribution is the presentation of a Lagrange series method for the characteristic polynomial $c_{A_G}(\lambda)$ to find the eigenvalues, in combination with the Interlacing theorem (see e.g. [10, p. 246]), that provides excellent expansion points for the Lagrange series. Here, we merely focus on the largest eigenvalue $\lambda_1$ of $A_G$, which is coined the spectral radius of the adjacency matrix $A_G$. Earlier in [9] and [11], we have deduced lower bounds for the spectral radius of a graph using Lagrange series.

∗Received by the editors on December 13, 2015. Accepted for publication on December 21, 2015. Handling Editor: Bryan L. Shader.
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We demonstrate the Lagrange series method on the kite graph $P_nK_m$ instead of their $PK_{n,m}$, to more clearly associate the index $n$ with the length of the path or number of nodes in $P_n$ and the index $m$ with the size of the clique $K_m$. We denote the spectral radius of the adjacency matrix of the kite $P_nK_m$ by $\lambda_1(P_nK_m)$. Stevanović and Hansen \cite{7} observe that $\lambda_1(P_0K_m) = m - 1$, but the analytic evaluation of $\lambda_1(P_nK_m)$ for $n > 0$ is not so easy. For any $m \geq 0$, they mention that $P_nK_m$ is a proper subgraph of $P_nK_{m+1}$ and, by the fact that the spectral radius is always larger than that of any of its subgraphs \cite{11}, the sequence $\{\lambda_1(P_nK_m)\}_{m \geq 0}$ is strictly increasing in $m$. Further, since $\lambda_1(P_nK_m) \leq d_{\text{max}}$ and $d_{\text{max}} = m$, we find the bounds

$$m - 1 \leq \lambda_1(P_nK_m) \leq m.$$  

Stevanović and Hansen \cite{7} present sharper bounds

$$m - 1 + \frac{1}{m^2} + \frac{1}{m^3} \leq \lambda_1(P_nK_m) \leq m - 1 + \frac{1}{4m} + \frac{1}{m^2 - 2m}. \quad (1.1)$$

In his recent book \cite{6}, Stevanović focuses in detail on the spectral radius of the infinitely long kite graph ($n \to \infty$), which is analytically computable \cite{7},

$$\lim_{n \to \infty} \lambda_1(P_nK_m) = \frac{m - 3 + \sqrt{(m + 1)^2 + \frac{4}{m^2 - 2}}}{2}.$$  

Cioabă and Gregory \cite{2}, whose notation $P_nK_m$ we have adopted, but not their name “lollipop” for the kite graph, prove the bounds

$$m - 1 + \frac{1}{m(m - 1)} \leq \lambda_1(P_nK_m) \leq m - 1 + \frac{1}{(m - 1)^2}. \quad (1.2)$$

Apart from introducing the name “lollipop” for $P_nK_m$, Brightwell and Winkler \cite{11} have proved that the maximum expected time for a random walk between two nodes is attained in a kite graph $P_nK_m$ of size $N = n + m - 1$ with $m = \lceil (2N - 2)/3 \rceil$.

Here, we derive the approximation (3.3) below, which lies – in most computed cases – between the above bounds in (1.1) and the sharper ones in (1.2).

2. The characteristic polynomial of the kite graph. The characteristic polynomial of the complete graph $K_m$ on $m$ nodes is

$$c_{AK_m}(\lambda) = (-1)^n(\lambda + 1)^n - (\lambda + 1 - n)$$

and that of the path $P_n$ on $n$ nodes is

$$c_{AP_n}(\lambda) = (-1)^n\frac{\sin \left( (n + 1) \arccos \frac{\lambda}{2} \right)}{\sin \left( \arccos \frac{\lambda}{2} \right)}.$$
Both are derived in [10, Chapter 5]. The zeros of \(c_{A_{P_n}}(\lambda)\), thus the eigenvalues of the adjacency matrix \(A_{P_n}\) of the path \(P_n\), are

\[
(\lambda_{P_n})_k = 2 \cos \frac{k \pi}{n + 1}
\]

for \(1 \leq k \leq n\). Since both \(K_m\) and \(P_n\) are subgraphs of the kite \(P_nK_m\), the Interlacing theorem (see e.g. [10, p. 246]) tells us that the eigenvalues of the adjacency matrix \(A_{P_k,n}\) of the kite lie in between the eigenvalues of \(A_{K_m}\) and \(A_{P_n}\). The explicit knowledge of the latter eigenvalues makes the presented Lagrange series approach particularly effective, as shown below.

To proceed, we need Theorem 2.1, which appears in Cvetković et al. [3, Section 2.3] and is attributed to Heilbronner [4]:

**Theorem 2.1.** The characteristic polynomial \(c_{A_G}(\lambda)\) of the adjacency matrix \(A_G\) of the graph \(G\) consisting of two disjoint graphs \(G_1\) and \(G_2\) connected by a link between the nodes \(i \in G_1\) and \(j \in G_2\) is

\[
c_{A_G}(\lambda) = \det (A_G - \lambda I) = \det (A_{G_1} - \lambda I) \det (A_{G_2} - \lambda I) - \det (A_{G_1 \setminus \{i\}} - \lambda I) \det (A_{G_2 \setminus \{j\}} - \lambda I).
\]

Theorem 2.1 applied to the kite \(P_nK_m\), yields

\[
c_{A_{P_nK_m}}(x) = \frac{2(x + 1)^{m-2}r(n, m; x)}{(-1)^{m+n}\sqrt{4 - x^2}},
\]

where

\[
r(n, m; x) = (m-x-2)\sin \left(n \arccos \left(\frac{x}{2}\right)\right) + (x+1)(1-m+x)\sin \left((n+1) \arccos \left(\frac{x}{2}\right)\right).
\]

The eigenvalues of the kite \(P_nK_m\), apart from the trivial \(x = -1\) with multiplicity \(m - 2\), satisfy

\[
r(n, m; x) = 0
\]

but cannot be \(x = \pm 2\) (due to the omission of the denominator in (2.3)).

The explicit form (2.3) shows that, since \(c_{A_{P_nK_m}}(0) = (-1)^{m+n-1} (m-1)\) for even \(n\), but \(c_{A_{P_nK_m}}(0) = (-1)^{m+n-1} (m-2)\) for odd \(n\), the adjacency matrix \(A_{P_nK_m}\) is invertible for \(m > 2\). Another observation for \(x = -1\) shows, with \(\arccos \left(\frac{1}{2}\right) = \pm \frac{\pi}{3} + 2k\pi\), that (2.3) reduces to \((m-1)\sin \left(\frac{\pi}{2}\right) = 0\), which is possible when \(n\) is a multiple of 3. In conclusion, the multiplicity of the eigenvalue \(-1\) of \(c_{A_{P_k,n}}(x)\) is \(m - 2\) when \(n\) is not a multiple of \(m\), otherwise the multiplicity of \(-1\) is \(m - 1\).
Let $\theta = \arccos \left( \frac{x}{2} \right)$ so that $x = 2 \cos \theta$. Obviously, when $\theta = iy$ is imaginary, then $x = 2 \cosh y \geq 2$ for any real $y$. We rewrite (2.5) with (2.4) as

$$(m - x - 2) \sin (n\theta) - (m - x - 1)(x + 1) \sin ((n + 1)\theta) = 0,$$

or

$$0 = (m - x - 1) \sin (n\theta) - (m - x - 1)(x + 1) \sin ((n + 1)\theta)$$

Introducing $x = 2 \cos \theta$ yields

$$0 = (m - 2 \cos \theta - 1) \{ \sin (n\theta) - (2 \cos \theta + 1) \sin ((n + 1)\theta) \} - \sin (n\theta)$$

For large $m$, we observe that $(m - 1 - 2 \cos \theta) \to 0$ or $x \to m - 1$.

### 3. The Lagrange series for the zero $\zeta (\theta_0)$ of $f (\theta)$ close to $\theta_0$. Consider the entire function $f (\theta)$ in $\theta$ in (2.6), whose largest real zero we aim to derive by Lagrange series [10, p. 304–305] using our characteristic coefficients [8]. The analysis of Stevanović and Hansen [7] shows that $\lambda_1 (P_n K_m)$ is close to $m - 1$, suggesting to expand $f (\theta)$ in a Taylor series around $\theta_0 = \arccos \left( \frac{m - 1}{2} \right)$, which is explicitly given in Appendix A.

The zero $\zeta (\theta_0)$ of $f (\theta)$ obeys $f (\zeta (\theta_0)) = 0$ and can be computed to any level of accuracy by Lagrange series expansion [12]. By using our characteristic coefficients and their underlying recursion (see [8] and [9]), the Lagrange series around $\theta_0$ can be elegantly executed (symbolically) to any desired accuracy only assuming the knowledge of the Taylor coefficients $f_k (\theta_0)$ around $\theta_0$ of

$$f (\theta) = \sum_{k=0}^{\infty} f_k (\theta_0) (\theta - \theta_0)^k.$$

We refer to Rivlin [5] for properties of the Chebyshev polynomials $T_n (x) = \cos n \arccos x = \cosh n \arccosh x$. 

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Explicitly up to order five, the zero $\zeta(\theta_0)$ around $\theta_0$ is presented as a Lagrange series in $z = \frac{f_0(\theta_0)}{f_1(\theta_0)}$ in [S], [[10] p. 304–305] as

$$\zeta(\theta_0) \approx \theta_0 - z - \frac{f_2(\theta_0)}{f_1(\theta_0)} z^2 + \left[ -2 \frac{f_2(\theta_0)}{f_1(\theta_0)} + \frac{f_3(\theta_0)}{f_1(\theta_0)} \right] z^3$$

$$+ \left[ -5 \frac{f_2(\theta_0)}{f_1(\theta_0)} + 5 \frac{f_3(\theta_0)}{f_1(\theta_0)} \right] z^4 + \left[ -14 \frac{f_2(\theta_0)}{f_1(\theta_0)} + 21 \frac{f_3(\theta_0)}{f_1(\theta_0)} \right] z^5. \quad (3.1)$$

Since $f_0(\theta_0) = f(\theta_0)$ and $f_1(\theta_0) = f'(\theta_0) = \frac{df(\theta)}{d\theta} |_{\theta = \theta_0}$, the Lagrange series up to first order in $z = \frac{f(\theta_0)}{f_1(\theta_0)}$, thus $\zeta(\theta_0) = \theta_0 - \frac{f(\theta_0)}{f_1(\theta_0)} + O(z^2)$ is equal to the Newton-Raphson approximation at $\theta = \theta_0$. From Appendix A, the first order term $z$ in the Lagrange series for the zero $\zeta(\theta_0)$ of $f(\theta)$ is

$$z = \frac{f_0(\theta_0)}{f_1(\theta_0)} = \frac{RG_0 + \sin (n\theta_0)}{\cos (n\theta_0) n + 2 \sin (\theta_0) G_0 - R \{ \cos ((n + 2) \theta_0) (n + 2) + \cos ((n + 1) \theta_0) (n + 1) \}} \quad (3.2)$$

with $R = m - 1 - 2 \cos \theta_0$ and $G_0 = \sin ((n + 2) \theta_0) + \sin ((n + 1) \theta_0)$.

If we are able to formally compute all Taylor coefficients of $f(\theta)$ (as here in Appendix A) in terms of an arbitrary expansion point $\theta_0$, then all zeros of $f(\theta)$ can be presented by (3.1) up to order 5 and higher orders [9] [8], that converges towards the zero $\zeta(\theta_0)$ of $f(\theta)$ closest to $\theta_0$. All eigenvalues of the adjacency matrix of the kite, except for the second largest, then follow as $\lambda_k(P_nK_m) = 2 \cos \zeta(\theta_{0,k})$, where the expansion point $\theta_{0,k}$ for the $k$-th largest eigenvalue $\lambda_k(P_nK_m)$ can be deduced from the Interlacing theorem (see e.g. [10] p. 246), that provides bounds for the eigenvalues, which are usually excellent estimates for the expansion point $\theta_0$. The Interlacing theorem tells us that the second largest eigenvalue $\lambda_2(P_nK_m)$ is smaller than 2. However, $\theta_0 = \arccos \left(\frac{1}{2}\right) = \pi$ and $f(\pi) = 0$, because in [28], that led to $f(\theta)$, the denominator $\sqrt{4 - x^2}$ in [28] has been ignored. Hence, the characteristic polynomial [28] indicates that $x = 2$ and $x = -2$ cannot be eigenvalues of the adjacency matrix of the kite $P_nK_m$. The situation can be remediated, precisely as in [8], which we omit here; the other choice is to deduce an appropriate expansion point $\theta_{0,2} < \pi$.

When $z = \frac{f_0(\theta_0)}{f_1(\theta_0)}$ is small, implying that the expansion point $\theta_0$ is close to the
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zero \( \zeta(\theta_0) \), the first order term in (3.1) is accurate and

\[
\lambda_k(P_n K_m) \approx 2 \cos((\theta_{0,k}) - z) = 2 \cos(\theta_{0,k}) \cos z + 2 \sin(\theta_{0,k}) \sin z
\]

\[
\approx 2 \cos(\theta_{0,k}) \left(1 - \frac{z^2}{2}\right) + 2 \sin(\theta_{0,k}) + O(z^3).
\]

Up to order \( O(z^2) \), we obtain a first order estimate for the \( k \)-th largest eigenvalue of the kite,

\[
\lambda_k(P_n K_m) \approx 2 \cos(\theta_{0,k}) + 2 \sin(\theta_{0,k}) + O(z^2)
\]

given \( \theta_{0,k} \). Guided by the Interlacing theorem and (2.1), we propose \( \theta_{0,k} = \frac{k\pi}{n+1} \) for \( 1 < k \leq n \) and \( \cos(\theta_{0,1}) = \frac{m-1}{n} \). Numerical computations, based on these expansion points, reveal that only a few terms in the Lagrange series suffice for \( \lambda_2(P_n K_m) \), except for small \( n \). The accuracy is worst for \( n = 1 \) as also follows from (3.2), but this case is analytically tractable [7].

In the remainder, we confine ourselves to the largest eigenvalue of the kite graph \( \lambda_1(P_n K_m) = 2 \cos(\zeta(\theta_{0,1})) \) with \( \theta_{0,1} = \arccos \left(\frac{m-1}{2}\right) \). Since \( R = m - 1 - 2 \cos\theta_0 = 0 \), the general expression (3.2) for \( z \) simplifies to

\[
z = \frac{f_0(\theta_{0,1})}{f_1(\theta_{0,1})} = \frac{\sin(n\theta_{0,1})}{2\sin((n+2)\theta_{0,1}) + \sin((n+1)\theta_{0,1})}\sin(\theta_{0,1}) + \cos(n\theta_{0,1})n.
\]

Moreover, for \( m > 1 \), \( \cos(\theta_{0,1}) = \frac{m-1}{2} \) implies that \( \theta_{0,1} \) is imaginary (and also \( z \)). Hence, with \( \cosh(\theta_{0,1}) = \frac{m-1}{2} \), \( i \sinh(\theta_{0,1}) = \sqrt{(\frac{m-1}{2})^2 - 1} \) and \( \theta_{0,1} = \cosh^{-1}(\frac{m-1}{2}) \), the spectral radius of the kite \( P_n K_m \) is approximated up to order \( O(z^2) \) by

\[
\lambda_1(P_n K_m) \approx (m - 1) + \frac{2 \sinh(n\theta_{0,1})}{2\sinh((n+2)\theta_{0,1}) \sinh((n+1)\theta_{0,1}) + \cosh(n\theta_{0,1}) \frac{n}{\sqrt{(\frac{m-1}{2})^2 - 1}}}. \tag{3.3}
\]

For a given \( n \), numerical computations revealed that this first order term (3.3) is increasingly accurate for increasing \( m \) and generally more accurate than the bound in (1.1) as well as in (1.2). Of course, when incorporating more terms in the Lagrange expansion a higher accuracy can be attained, but we found that the first term (3.3) alone was already surprisingly accurate. The table below compares several approximations of \( \lambda_1(P_n K_m) - (m - 1) \) for \( n = 20 \). Only when \( m \) is small compared to \( n \), the Lagrange expansion leads to less accurate results.
The method can be applied as well to the combination of the star and the path graph and, in principle, to any graph, whose characteristic polynomial is known, provided also a good approximation of the expansion point (like $\theta_0$), e.g. by interlacing, is available so that the Lagrange series rapidly converges.

Appendix A. Taylor expansion of $f(\theta)$ around $\theta_0$.

It is convenient in the function $f(\theta)$, defined in (2.6), to write the argument explicitly in terms of the expansion point $\theta_0$, as

$$\theta = \theta_0 + \theta - \theta_0 = \theta_0 + y$$

with $y = \theta - \theta_0$, so that

$$f(\theta) = - (m - 2 \cos(\theta_0 + y) - 1) [\sin((n + 2)(\theta_0 + y)) + \sin((n + 1)(\theta_0 + y))]$$

$$- \sin(n(\theta_0 + y)) .$$

The Taylor expansion of $f(\theta)$ around $\theta_0$ is

$$f(\theta) = \sum_{k=0}^{\infty} f_k(\theta_0) y^k ,$$

where the Taylor coefficients $f_k(\theta_0)$ now need to be computed.

With the elementary identity $\cos(\theta_0 + y) = \cos(\theta_0) \cos(y) - \sin(\theta_0) \sin(y)$, we have that

$$(m - 2 \cos \theta - 1) = m - 1 - 2 \cos(\theta_0) \cos(y) + 2 \sin(\theta_0) \sin(y)$$

$$= m - 1 - \sum_{k=0}^{\infty} (-1)^k \frac{2 \cos(\theta_0) y^{2k}}{(2k)!} + \sum_{k=0}^{\infty} (-1)^k \frac{2 \sin(\theta_0) y^{2k+1}}{(2k+1)!} .$$

In order to ease the Cauchy product below, we write the right-hand side as one Taylor series in $y^k$,

$$(m - 2 \cos \theta - 1) = \sum_{k=0}^{\infty} b_k y^k .$$
with \( b_0 = m - 1 - 2 \cos \theta_0 \) and, for \( k > 0 \),

\[
 b_k = \begin{cases} 
 -2 \cos (\theta_0), & \text{if } k \text{ is even}, \\
 \frac{1}{2} (2 \sin (\theta_0)), & \text{if } k \text{ is odd}.
\end{cases}
\]

Similarly, using \( \sin (q (\theta_0 + y)) = \sin (q \theta_0) \cos (q y) + \cos (q \theta_0) \sin (q y) \),

\[
 G = \sin ((n + 2) \theta) + \sin ((n + 1) \theta)
 = \sin ((n + 2) \theta_0) \cos ((n + 2) y) + \cos ((n + 2) \theta_0) \sin ((n + 2) y) + \sin ((n + 1) \theta_0) \cos ((n + 1) y) + \cos ((n + 1) \theta_0) \sin ((n + 1) y)
 = \sin ((n + 2) \theta_0) \sum_{k=0}^{\infty} (-1)^k \frac{(n + 2)^{2k} y^{2k}}{(2k)!}
 + \cos ((n + 2) \theta_0) \sum_{k=0}^{\infty} (-1)^k \frac{(n + 2)^{2k+1} y^{2k+1}}{(2k+1)!}
 + \sin ((n + 1) \theta_0) \sum_{k=0}^{\infty} (-1)^k \frac{(n + 1)^{2k} y^{2k}}{(2k)!}
 + \cos ((n + 1) \theta_0) \sum_{k=0}^{\infty} (-1)^k \frac{(n + 1)^{2k+1} y^{2k+1}}{(2k+1)!}
\]

and

\[
 G = \sin ((n + 2) \theta) + \sin ((n + 1) \theta)
 = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} \left\{ \sin ((n + 2) \theta_0) (n + 2)^{2k} + \sin ((n + 1) \theta_0) (n + 1)^{2k} \right\} y^{2k}
 + \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \left\{ \cos ((n + 2) \theta_0) (n + 2)^{2k+1} + \cos ((n + 1) \theta_0) (n + 1)^{2k+1} \right\} y^{2k+1},
\]

which we write as one Taylor series in \( y^k \)

\[
 \sin ((n + 2) \theta) + \sin ((n + 1) \theta) = \sum_{k=0}^{\infty} \frac{i^k}{k!} a_k y^k,
\]

where

\[
 a_k = \begin{cases} 
 \sin ((n + 2) \theta_0) (n + 2)^k + \sin ((n + 1) \theta_0) (n + 1)^k, & \text{if } k \text{ is even}, \\
 \frac{1}{2} \left( \cos ((n + 2) \theta_0) (n + 2)^k + \cos ((n + 1) \theta_0) (n + 1)^k \right), & \text{if } k \text{ is odd}.
\end{cases}
\]

Let us denote the first term in \( f (\theta) \) in (2.6) by

\[
 h (\theta) = (m - 2 \cos (\theta) - 1) \{ \sin ((n + 2) \theta) + \sin ((n + 1) \theta) \}. 
\]
Then the Cauchy product is
\[ h(\theta) = \sum_{k=0}^{\infty} i_k^k b_k y^k = \sum_{k=0}^{\infty} \sum_{s=0}^{k} \frac{i^s}{s!} a_s y^s b_{k-s} y^k \]
\[ = \sum_{k=0}^{\infty} \left\{ \sum_{s=0}^{k} \frac{k^k}{s!} a_s b_{k-s} \right\} y^k. \]

Finally, we arrive at the Taylor series of \( f(\theta) \) around \( \theta_0 \),
\[ f(\theta) = -\sum_{k=0}^{\infty} \left\{ \frac{i^k}{k!} \left( \sum_{s=0}^{k} \frac{k^k}{s!} a_s b_{k-s} + c_k \right) \right\} y^k, \]
where the coefficient \( c_k \) is of similar type as \( a_k \),
\[ c_k = \begin{cases} \sin(n \theta_0) n^k, & k \text{ even,} \\ \frac{1}{n} \cos(n \theta_0) n^k, & k \text{ odd,} \end{cases} \]
from which we find the Taylor coefficients of \( f(\theta) \) around \( \theta_0 \) as
\[ f_k(\theta_0) = -\frac{i^k}{k!} \left( \sum_{s=0}^{k} \frac{k^k}{s!} a_s b_{k-s} + c_k \right). \]

The first two terms are
\[ f_0(\theta_0) = f(\theta_0) \]
\[ = -(m-1-2 \cos \theta_0) \{ \sin ((n+2) \theta_0) + \sin ((n+1) \theta_0) \} \]
and
\[ f_1(\theta_0) = -\cos(n \theta_0) n - 2 \sin(\theta_0) \{ \sin ((n+2) \theta_0) + \sin ((n+1) \theta_0) \} \]
\[ (m-1-2 \cos \theta_0) \{ \cos ((n+2) \theta_0) (n+2) + \cos ((n+1) \theta_0) (n+1) \}. \]

REFERENCES


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