INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 5, Number 3, Pages 457–465

EXPLICIT HERMITE INTERPOLATION POLYNOMIALS VIA THE CYCLE INDEX WITH APPLICATIONS

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Abstract. The cycle index polynomial of a symmetric group is a basic tool in combinatorics and especially in Pólya enumeration theory. It seems irrelevant to numerical analysis. Through Faá di Bruno's formula, cycle index is connected with numerical analysis. In this work, the Hermite interpolation polynomial is explicitly expressed in terms of cycle index. Applications in Gauss-Turán quadrature formula are also considered.

Key Words. symmetric group, cycle index polynomial, Faá di Bruno's formula, Bell's polynomial, Hermite interpolation polynomial, Gauss-Turán quadrature formula.

1. Introduction

The cycle index polynomial of a symmetric group is a basic tool in combinatorics and plays an important role in Pólya enumeration theory. It is seemingly irrelevant to numerical analysis. To our best knowledge, its applications in numerical analysis is not systematical and many of them are in its disguises, see e.g., [16, 17, 21]. Actually, it can have wide applications in numerical analysis. Using cycle index polynomial, [19] find a closed form solution for a nonlinear system of equations, a problem arising in constructing nonlinear best quadrature formulas for Sobolev classes [18]. A further development and the proof of [19] are contained in [20].

As is well known, Faá di Bruno's formula applies when explicit higher derivatives of a composite function are sought [4]. Bell's polynomial arises naturally in Faá di Bruno's formula. The former is closely related to the cycle index polynomial. Therefore, it turns up in problems where higher derivatives of a composite function or its variants are involved. Algebraic and combinatorial tools and techniques can be exploited in such problems, which make analysis and computations easily accessible.

Based on Faá di Bruno's formula and logarithmic differentiation, the Hermite interpolation polynomial is explicitly expressed in terms of cycle index in this paper. And so are the divided differences with multiplicity. To our best knowledge, these formulas are new. Applications of these formulas to Gauss-Turan quadrature formulas are also included.

This work focuses on explicit Hermite interpolation polynomials via the cycle index, aiming at stimulating more attention to applications of the cycle index in numerical analysis.

Received by the editors November 11, 2006 and, in revised form, July 2, 2007.
2000 *Mathematics Subject Classification.* 05A15, 65D05, 65D32.

2. Cycle index of symmetric group and Hermite interpolation polynomial

Throughout, let $[n] := \{1, 2, \ldots, n\}$ and $\mathfrak{G}$ be a permutation group of degree n. For any permutation $\sigma \in \mathfrak{G}$ and $i \in [n]$, let $c_i(\sigma)$ be the number of cycles of length of i in σ. The key result of Pólya theory is an expression for the number of orbits in terms of the cycle index polynomial of $\mathfrak{G}$. This polynomial, in n variables, is defined as follows [4, 10].

Definition 2.1.

$$Z(\mathfrak{G}; x_1, x_2, \ldots, x_n) := \frac{1}{|\mathfrak{G}|} \sum_{\sigma \in \mathfrak{G}} x_1^{c_1(\sigma)} x_2^{c_2(\sigma)} \cdots x_n^{c_n(\sigma)}, \tag{2.1}$$

where $|\mathfrak{G}|$ is the order of $\mathfrak{G}$, i.e., the number of its elements. If $\mathfrak{G}$ =symmetric group $\mathfrak{S}_n$ of degree n, then its cycle index polynomial is written as

$$Z_n(x_1, x_2, \ldots, x_n) := Z(\mathfrak{S}_n; x_1, x_2, \ldots, x_n). \tag{2.2}$$

The following lemma can be easily verified (cf. [20]).

Lemma 2.2. (Recurrence relation)

$$\begin{aligned} &Z_0 = 1, \\ &n Z_n(x_1, x_2, \ldots, x_n) = \sum_{k=1}^{n} x_k Z_{n-k}(x_1, x_2, \ldots, x_{n-k}),\ n \geq 1. \end{aligned} \tag{2.3}$$

Here are first few examples of cycle index

$$\begin{aligned} Z_1(x_1) &= x_1, \\ Z_2(x_1, x_2) &= \frac{1}{2}(x_1^2 + x_2), \\ Z_3(x_1, x_2, x_3) &= \frac{1}{6}(x_1^3 + 3x_1x_2 + 2x_3), \\ Z_4(x_1, x_2, x_3, x_4) &= \frac{1}{24}(x_1^4 + 6x_1^2x_2 + 3x_2^2 + 8x_1x_3 + 6x_4). \end{aligned}$$

For convenience, we write

$$Z_n(x_k) := Z_n(x_k \mid k \in [n]) := Z_n(x_1, x_2, \ldots, x_n).$$

Related to cycle index is Bell's polynomial which arises naturally in explicit expressions for high-order derivatives of a composite function. The following is (exponential) complete Bell's polynomial

$$Y_n(x_k) := Y_n(x_k \mid k \in [n]) := n! Z_n\Big(\frac{x_k}{(k-1)!} \mid k \in [n]\Big), \tag{2.4}$$

which can also be expressed as the sum of exponential partial Bell's polynomials $B_{n,m}$

$$Y_n(x_k) = \sum_{m=1}^{n} B_{n,m}(x_k).$$

Here

$$B_{n,m}(x_k | k \in [n]) := \sum_{\substack{a_1+2a_2+\cdots+na_n=n \\ a_1+a_2+\cdots+a_n=m}} \frac{n!}{a_1!(1!)^{a_1} a_2!(2!)^{a_2} \cdots a_n!(n!)^{a_n}} x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n}.$$

Bell's polynomials appear in Faá di Bruno's formula which explicitly gives the high-order derivatives of the composite function $g \circ f$ of functions g and f [4].

Lemma 2.3. (Faá di Bruno's Formula)

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} g(f(t)) = \sum_{m=1}^{n} g^{(m)}(f(t)) B_{n,m}(f^{(k)}(t) | k \in [n]), \tag{2.5}$$

in particular,

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} \exp(f(t)) = \exp(f(t)) Y_n(f^{(k)}(t) \mid k \in [n]). \tag{2.6}$$

From (2.4) and (2.6) follows

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} \exp(f(t)) = n! \exp(f(t)) Z_n\Big(\frac{f^{(k)}(t)}{(k-1)!} \mid k \in [n]\Big). \tag{2.7}$$

Suppose $x_1, x_2, \ldots, x_n$ are different and we are given data $f^{(j)}(x_i),\ i = 1, 2, \ldots, n; j = 0, 1, \ldots, m_i - 1$, where m_i are natural numbers. The Hermite interpolation problem is to find a polynomial of least degree $N := \sum_{i=1}^{n} m_i - 1$ satisfying

$$H^{(j)}(x_i) = f^{(j)}(x_i), \quad i = 1, 2, \ldots, n;\ j = 0, 1, \ldots, m_i - 1. \tag{2.8}$$

This polynomial, called Hermite interpolation polynomial, is known to be unique and can be expressed as [2] (cf. [24], but there exist some typos.)

$$H(x) = \sum_{i=1}^{n} \sum_{j=0}^{m_i-1} f^{(j)}(x_i) \sum_{k=0}^{m_i-j-1} \frac{1}{j!k!} \Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)^{(k)}_{x=x_i} \frac{\Omega(x)}{(x-x_i)^{m_i-j-k}}, \tag{2.9}$$

where

$$\Omega(x) = \prod_{i=1}^{n} (x - x_i)^{m_i}.$$

It seems that there is no explicit expressions available for

$$\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)^{(k)}_{x=x_i}.$$

The first aim here is to give a closed form for it in terms of the cycle index. This may help us gain some insight into the structure of the Hermite interpolation polynomial. As a consequence, an explicit expression for the divided difference with multiplicity of a function is also derived.

Now, set

$$g_i(x) := \log\left|\frac{(x-x_i)^{m_i}}{\Omega(x)}\right|. \tag{2.10}$$

Then we have

$$g_i(x) := -\sum_{l \neq i} m_l \log|x - x_l|, \tag{2.11}$$

and it is easy to verify

$$g_i^{(r)}(x) := (-1)^r (r-1)! \sum_{l \neq i} \frac{m_l}{(x - x_l)^r}. \tag{2.12}$$

This together with (2.7) yields

Lemma 2.4. *Symbols are as above.*

$$\frac{1}{k!}\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)^{(k)} = \frac{(x-x_i)^{m_i}}{\Omega(x)} Z_k\Big((-1)^r \sum_{l\neq i} \frac{m_l}{(x-x_l)^r}\Big| r\in[k]\Big).$$

In particular,

$$\frac{1}{k!}\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)^{(k)}_{x=x_i} = \prod_{l\neq i}(x_i-x_l)^{-m_l} Z_k\Big((-1)^r \sum_{l\neq i} \frac{m_l}{(x_i-x_l)^r}\Big| r\in[k]\Big).$$

Proof. It suffices to prove the first assertion. A straightforward calculation on using (2.7) yields

$$\begin{aligned}\frac{1}{k!}\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)^{(k)} &= \frac{1}{k!}\frac{\mathrm{d}^k}{\mathrm{d}x^k}\exp(g_i(x))\mathrm{sgn}\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)\\ &= \exp(g_i(x))Z_k\Big(\frac{g_i^{(r)}(x)}{(r-1)!} \mid r\in[k]\Big)\mathrm{sgn}\Big(\frac{(x-x_i)^{m_i}}{\Omega(x)}\Big)\\ &= \frac{(x-x_i)^{m_i}}{\Omega(x)} Z_k\Big(\frac{g_i^{(r)}(x)}{(r-1)!} \mid r\in[k]\Big),\end{aligned}$$

which combined with (2.12) gives the first assertion. □

From Lemma 2.4 and (2.8), we readily have (cf. [15])

Theorem 2.5. *The Hermite interpolation polynomial solving problem* (2.8) *is given by*

(2.13)

$$H(x) = \sum_{i=1}^{n}\sum_{j=0}^{m_i-1} \frac{f^{(j)}(x_i)}{j!} \prod_{l\neq i}\Big(\frac{x-x_l}{x_i-x_l}\Big)^{m_l} \sum_{k=j}^{m_i-1}(x-x_i)^k Z_{k-j}\Big(\sum_{l\neq i}\frac{m_l}{(x_l-x_i)^r}\Big| r\in[k-j]\Big).$$

In particular, if $m_1 = m_2 = \ldots = m_n = m$, *then*

(2.14)

$$H(x) = \sum_{i=1}^{n}\sum_{j=0}^{m-1} \frac{f^{(j)}(x_i)}{j!}\ell_i(x)^m \sum_{k=j}^{m-1}(x-x_i)^k Z_{k-j}\Big(\sum_{l\neq i}\frac{m}{(x_l-x_i)^r}\Big| r\in[k-j]\Big),$$

where

$$\ell_i(x) = \prod_{l\neq i}\frac{x-x_l}{x_i-x_l}$$

is the ith Lagrange interpolation basis function.

The case of $m_1 == m_2 = \ldots = m_n = m$ was also addressed in [12]. By a partial fraction expansion, (2.14) was expressed in terms of Bell's polynomials.

If $m_i = 1$ for any i, then $k = j = 0$, and the above formula reproduces the Lagrange interpolation polynomial since in this case $Z_0 = 1$.

Let $f[x_1^{m_1}, x_2^{m_2}, \ldots, x_n^{m_n}]$ be the divided differences of the function f at points $x_1, x_2, \ldots, x_n$ with x_i repeated m_i times. It is clear that $f[x_1^{m_1}, x_2^{m_2}, \ldots, x_n^{m_n}]$ is the (highest) N degree coefficient in x contained in $H(x)$. With this in mind and the explicit expression (2.13) for $H(x)$, we immediately have

Corollary 2.6. *Suppose f is sufficiently smooth and $x_1, x_2, \ldots, x_n$ are different.*

$$\begin{aligned} f[x_1^{m_1}, x_2^{m_2}, \ldots, x_n^{m_n}] &= \sum_{i=1}^{n} \sum_{j=0}^{m_i-1} \frac{f^{(j)}(x_i)}{j! \prod_{l \neq i}(x_i - x_l)^{m_l}} \\ & \quad Z_{m_i-j-1}\Big((-1)^r \sum_{l \neq i} \frac{m_l}{(x_i - x_l)^r} \Big| r \in [m_i - j - 1]\Big). \end{aligned}$$

If, in particular, $m_1 = m_2 = \ldots = m_n = m$, then we have

$$\begin{aligned} f[x_1^{m}, x_2^{m}, \ldots, x_n^{m}] &= \sum_{i=1}^{n} \sum_{j=0}^{m-1} \frac{f^{(j)}(x_i)}{j! \prod_{l \neq i}(x_i - x_l)^{m}} \\ & \quad Z_{m-j-1}\Big((-1)^r \sum_{l \neq i} \frac{m}{(x_i - x_l)^r} \Big| r \in [m - j - 1]\Big). \end{aligned}$$

An expression in terms of Bell's polynomial for $f[x_1^m, x_2^m, \ldots, x_n^m]$ can be found in [12]. Both of the above formulas generalize the classical result

$$f[x_1, x_2, \ldots, x_n] = \sum_{i=1}^{n} \frac{f(x_i)}{\prod_{l \neq i}(x_i - x_l)}.$$

In the case of $m_1 = m_2 = \ldots = m_n = m$, another alternative approach for representing the Hermite interpolation polynomial can be described as follows. The difference of a function and its Lagrange interpolation vanishes at the interpolation nodes and therefore by Newton's formula

$$f(x) - \sum_{i=1}^{n} f(x_i)\ell_i(x) = f[x_1, x_2, \ldots, x_n, x]\omega(x), \tag{2.15}$$

where $\omega(x) = \prod_{i=1}^{n}(x - x_i)$ is the node polynomial. Applying (2.15) to function $f[x_1, x_2, \ldots, x_n, x]$ in x leads to

$$f[x_1, x_2, \ldots, x_n, x] - \sum_{i=1}^{n} f[x_1, x_2, \ldots, x_n, x_i]\ell_i(x) = f[x_1^2, x_2^2, \ldots, x_n^2, x]\omega(x).$$

Repeated applications of (2.15) to $f[x_1^2, x_2^2, \ldots, x_n^2, x], \ldots, f[x_1^{m-1}, x_2^{m-1}, \ldots, x_n^{m-1}, x]$ and rearrangement finally arrive at

$$H(x) = \sum_{i=1}^{n} \sum_{j=0}^{m-1} f[x_1^j, x_2^j, \ldots, x_n^j, x_i]\ell_i(x)\omega(x)^j. \tag{2.16}$$

This can be found in [3]. The divided difference term in (2.16) can be further expanded by Corollary 2.6, but we omit the details here.

3. Applications in Gauss-Turán quadrature

The Hermite interpolation polynomial is useful in constructing quadrature formulas including derivative information. Generally, replacing an integrand by (2.13) leads to a quadrature formula.

We now turn to consider quadrature formulas of Gauss type. More than one hundred years after Gauss, Turán [13] considered quadrature rules of the form

$$\int_{-1}^{1} f(x)w(x)\mathrm{d}x = \sum_{i=1}^{n} \sum_{j=0}^{2s} \lambda_{ij}(w) f^{(j)}(x_{i,s}) + R(f) \tag{3.1}$$

and showed that such rules have a maximum degree of precision $2(s+1)n-1$, that is, $R(f)=0$ if f is a polynomial of degree not exceeding $2(s+1)n-1$. Moreover, he showed that $x_{i,s}$ are the n zeros of the monic polynomial $p_n(x)$ of degree n which minimizes the following integral

$$\int_{-1}^{1} |p(x)|^{2s+2} w(x) \mathrm{d}x, \tag{3.2}$$

where

$$p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0.$$

Such polynomials are known as s-orthogonal polynomials with respect to the weight w and correspondingly (3.1) is called Gauss-Turán Quadrature formula.

By a theorem of Bernstein [1] the n-th Chebyshev polynomial of the first kind $2^{1-n}T_n(x)$ is the solution of (3.2) with respect to the Chebyshev weight $1/\sqrt{1-x^2}$. Yet despite this, little is known about the corresponding Cotes coefficients of high order. So Turán raised the following problem in this direction [14].

Problem 26. Give an explicit formula for $\lambda_{ij} := \lambda_{ij}(w)$ when $w = 1/\sqrt{1-x^2}$ and determine its asymptotic behavior as $n \to \infty$ and s is fixed.

Micchelli and Sharma [7] solved Turán's Problem 26. For a different approach, see [11]. As noted in [22], the following result of a 1972 paper by Micchelli and Rivlin [6]

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} \mathrm{d}x = \frac{\pi}{n} \Big\{ \sum_{i=1}^{n} f(x_i) + \sum_{\nu=1}^{s} \frac{1}{2\nu 4^{\nu n}} \binom{2\nu}{\nu} f'[x_1^{2\nu}, x_2^{2\nu}, \ldots, x_n^{2\nu}] \Big\} \tag{3.3}$$

is in fact a solution to Turán's Problem 26. Here, and throughout this section, $x_1, x_2, \ldots, x_n$ are the n zeros of T_n.

Generalizing and extending (3.3) and other related existing results, Gori and Micchelli [5] introduced and studied a class of weight functions which admit explicit Gauss-Turán Quadrature formulas. For every natural number n, the class, denoted by $\mathbb{W}_n$, consists of all positive integrable functions w on $[-1,1]$ such that

$$w(x)\sqrt{1-x^2} = \sum_{k=0}^{\infty}{}' \rho_k T_{2kn}(x), \tag{3.4}$$

where convergence holds with respect to the weighted L^1-norm

$$\int_{-1}^{1} |f(x)| \frac{\mathrm{d}x}{\sqrt{1-x^2}}.$$

Here the prime on the summation indicates that the first term is halved and f is defined and integrable on $[-1,1]$. They further showed among others that T_n is the n-th degree s-orthogonal polynomial relative to the weight function $w \in \mathbb{W}_n$.

As far as we know, apart from the weight $w \in \mathbb{W}_n$ admitting explicitly known s-orthogonal polynomial T_n there are only three other kinds of weights whose s-orthogonal polynomials are explicitly found (each of which depends on s), see Ossicini and Rosati [9] or consult [8]. As pointed out in [23], their corresponding quadrature formulas can be derived from the one corresponding to the weight $1/\sqrt{1-x^2}$, and therefore, essentially the only interesting case $w \in \mathbb{W}_n$ deserves investigation.

Now we consider any weight $w \in \mathbb{W}_n$. For $f \in C[-1,1]$ one obtains

$$I(f;w) := \int_{-1}^{1} f(x)w(x)\mathrm{d}x = \frac{\pi}{2} \sum_{k=0}^{\infty}{}' \rho_k A_{2kn}(f), \tag{3.5}$$

where $A_{kn}(f)$ are the Fourier-Chebyshev coefficients

$$A_{kn}(f) = \frac{2}{\pi}\int_{-1}^{1} f(x)T_{kn}(x)\frac{\mathrm{d}x}{\sqrt{1-x^2}}, \quad k = 0, 1, \ldots. \tag{3.6}$$

Let $\mathbb{N}$ be the set of all natural numbers, $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Using divided difference functionals at the Chebyshev nodes (with multiplicity), i.e., the zeros of T_n, Gori and Micchelli in [5] found explicit expressions for $A_{2kn}(f)$ and $A_{(2k+1)n}(f)$, $k \in \mathbb{N}_0$, respectively.

Later, one of us [22] provided an alternative approach to $I(f; w)$ and $A_{kn}(f)$. Also, the Cotes coefficients $\lambda_{ij}(w)$ were explicitly found in [22]. The approach can be outlined as follows. Taking $m = 2s + 1$ in (2.16) and substituting thus obtained Hermite interpolation polynomial $H(x)$ based on zeros T_n, one obtains

$$I(f; w) = I(H; w) = \sum_{i=1}^{n}\sum_{j=0}^{2s} \alpha_{ij}(w) f[x_1^j, x_2^j, \ldots, x_n^j, x_i] \tag{3.7}$$

has algebraic degree of exactness $2(s + 1)n - 1$, where

$$\alpha_{ij}(w) = \int_{-1}^{1} \ell_i(x)\omega(x)^j w(x)\mathrm{d}x.$$

It remains to find values of $\alpha_{ij}(w)$. A straightforward calculation using orthogonality finally yields

$$\alpha_{ij}(w) = \begin{cases} 0, & \text{if } j \text{ is odd;} \\ \dfrac{\pi}{2^{jn}n}\displaystyle\sum_{k=0}^{j/2}{}' \binom{j}{j/2-k}\rho_k, & \text{if } j \text{ is even.} \end{cases}$$

It is interesting to note that $\alpha_{ij}(w)$ is independent of i. Putting all together gives (3.8)

$$I(f; w) = \frac{\pi}{2n}\left\{\sum_{i=1}^{n} \rho_0 f(x_i) + \sum_{i=1}^{n}\sum_{j=1}^{s} \frac{2}{4^{jn}} \sum_{k=0}^{j}{}' \binom{2j}{j-k}\rho_k f[x_1^{2j}, x_2^{2j}, \ldots, x_n^{2j}, x_i]\right\}.$$

We pause to comment here the divided difference term in (3.8) can be expanded according to Corollary 2.6 to give explicit Cotes coefficients. Another way is as the original one in [22] on using the following fact due to [3]

$$\sum_{i=1}^{n} j f[x_1^j, x_2^j, \ldots, x_n^j, x_i] = f'[x_1^j, x_2^j, \ldots, x_n^j].$$

The above arguments lead to the following result due to [5]

$$I(f; w) = \frac{\pi}{2n}\left\{\sum_{i=1}^{n} \rho_0 f(x_i) + \sum_{j=1}^{s} \frac{1}{4^{jn}j} \sum_{k=0}^{j}{}' \binom{2j}{j-k}\rho_k f'[x_1^{2j}, x_2^{2j}, \ldots, x_n^{2j}]\right\}. \tag{3.9}$$

Now the divided difference term in (3.9) is expanded to yield the following main result in [22] (Now it is clear from Corollary 2.6 that (3.9) allows a direct expansion). The following Gauss-Turán quadrature formula

$$I(f; w) = \frac{\pi}{2n}\sum_{i=1}^{n}\left\{\rho_0 f(x_i) + \sum_{j=1}^{2s} \lambda_{ij}(w) f^{(j)}(x_i)\right\} \tag{3.10}$$

is exact for polynomial f of degree at most $2(s+1)n-1$, where

$$\lambda_{ij}(w) = \sum_{\nu=[\frac{j+1}{2}]}^{s} \frac{(1-x_i^2)^\nu b_{2\nu-j,i,2\nu}}{(j-1)!2^{2\nu}\nu n^{2\nu}} \sum_{k=0}^{\nu}{}' \binom{2\nu}{\nu-k}\rho_k \tag{3.11}$$

and

$$b_{kij} = \frac{1}{k!}(\ell_i(x)^{-j})^{(k)}_{x=x_i}, \quad k=0,1,\ldots; i=1,2,\ldots,n;\ j\in\mathbb{N}. \tag{3.12}$$

One comment is in order. The computation of b_{kij} is still not straightforward and thus deserves further effort. From Lemma 2.4, it follows

$$b_{kij} = Z_k\Big((-1)^r\sum_{l\neq i}\frac{j}{(x_i-x_l)^r}\Big| r\in[k]\Big), \quad k=0,1,\ldots; i=1,2,\ldots,n;\ j\in\mathbb{N}. \tag{3.13}$$

Therefore, (3.11) becomes

$$\lambda_{ij}(w) = \sum_{\nu=[\frac{j+1}{2}]}^{s} \frac{(1-x_i^2)^\nu}{(j-1)!2^{2\nu}\nu n^{2\nu}} Z_{2\nu-j}\Big((-1)^r\sum_{l\neq i}\frac{2\nu}{(x_i-x_l)^r}\Big| r\in[2\nu-j]\Big)$$

$$\sum_{k=0}^{\nu}{}' \binom{2\nu}{\nu-k}\rho_k. \tag{3.14}$$

This is more transparent than (3.11) with (3.12) and is more easily computed due to the recurrence relation in Lemma 2.2.

Acknowledgments

The authors thank the anonymous referee for his/her careful reading of the original manuscript.

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