HYPERGEOMETRIC SUMMATION ALGORITHMS FOR HIGH ORDER FINITE ELEMENTS

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Abstract. High order finite elements are usually defined by means of certain orthogonal polynomials. The performance of iterative solution methods depends on the condition number of the system matrix, which itself depends on the chosen basis functions. The goal is now to design basis functions minimizing the condition number, and which can be computed efficiently. In this paper we demonstrate the application of recently developed computer algebra algorithms for hypergeometric summation to derive cheap recurrence relations allowing a simple implementation for fast basis function evaluation.

1. Introduction

The finite element method (FEM) [14, 5, 6] is the most popular tool for the computer simulation of partial differential equations as arising from problems in science, engineering and economy.

The simplest method is to approximate the unknown functions by a continuous and piecewise linear function on a triangular mesh. To compute the function, one has to solve a usually large system of equations. For many problem classes, the approximation with piecewise high order polynomials requires essentially less parameters [13, 15], and is thus attractive. On the other hand, the implementation of high order methods is much more involved, and every simplification of algorithms is highly appreciated.

In particular for three dimensional problems, the dimension of the equation system gets large, and iterative equation solvers such as the preconditioned conjugate gradient method must be used. Our goal is to apply cheap block-Jacobi preconditioners, where each block consists of the unknowns connected with one vertex, edge, face, or cell of the mesh. To make this preconditioner efficient, the basis functions must be designed such that the blocks are nearly orthogonal among each other. The construction of such basis functions as well as the numerical analysis is given in [7]. Here, we concentrate on providing recursion formulas allowing a simple implementation for fast basis function evaluation. The main objective of this note is to show that recently developed computer algebra algorithms for special functions play a key role in this task. In Section 3 we present two examples which

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illustrate typical applications. Before entering this main part of the paper, in Section 2 we give a brief account of the computer algebra methods we apply.

2. Hypergeometric summation methods

All our summation methods applied in this article solve one of the following two problems.

• *The telescoping problem:* Given $f(k)$; find $g(k)$ such that

$$f(k) = g(k+1) - g(k)$$

holds within a certain range of k. Then, given such a $g(k)$, one derives by telescoping that

$$\sum_{k=1}^{n} f(k) = g(n+1) - g(1).$$

• *The creative telescoping problem:* Given $f(n,k)$ and a positive integer d; find $c_0(n)$, …, $c_d(n)$, free of k and not all zero, and $g(n,k)$ such that

$$c_0(n)\,f(n,k) + \cdots + c_d(n)\,f(n+d,k) = g(n,k+1) - g(n,k) \tag{1}$$

holds within a certain range of n and k. Suppose one succeeds in computing such $c_i(n)$ and $g(n,k)$ for given $f(n,k)$ and d. Then summing equation (1) over k from 1 to n gives

$$c_0(n)\sum_{k=1}^{n} f(n,k) + \cdots + c_d(n)\sum_{k=1}^{n} f(n+d,k) = g(n,n+1) - g(n,1). \tag{2}$$

Then under some mild extra conditions, one can express the sums $\sum_{k=1}^{n} f(n+i,k)$ in (2) in terms of $S(n+i)$ where $S(n) = \sum_{k=1}^{n} f(n,k)$. This implies a not necessarily homogeneous recurrence

$$c_0(n)S(n) + \cdots + c_d(n)S(n+d) = h(n) \tag{3}$$

for the definite sum $S(n)$.

For hypergeometric terms[1] $f(k)$ in k (resp. hypergeometric terms $f(n,k)$ in n and k) well-known algorithms exist, see e.g. [10]. More generally, new algorithms [12, 2] are on the market that can handle sequences where $f(k)$ (resp. $f(n,k)$) is defined by certain types of linear recurrence relations of higher order with respect to k.

For a broad variety of such algorithms, see

`http://www.risc.uni-linz.ac.at/research/combinat/software/`

However, for this article we restrict to our Mathematica package [12].

In[1]:= << **Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-Linz

Besides these summation methods we will have to deal also with the following problem.

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[1] $f(k)$ is hypergeometric in k iff $f(k+1)/f(k) = g(k)$ for some fixed rational function $g(k)$.

•*Manipulation of linear recurrences:* Given two linear recurrence relations, one as in (3) and one of the form

$$b_0(n)R(n) + \cdots + b_r(n)R(n+r) = g(n),$$

both with polynomial coefficients $b_i(n)$ and $c_i(n)$; find a recurrence relation of the same type which is satisfied by the sum sequence $R(n) + S(n)$.

Also here there exist various algorithms that can solve this problem, see [11, 8]. In this article we use our Mathematica package [8].

In[2]:= **<< GeneratingFunctions.m**
GeneratingFunctions Package by Christian Mallinger – © RISC Linz

3. Two examples from high order finite elements

In this section we present two examples arising from the design of high order finite elements.

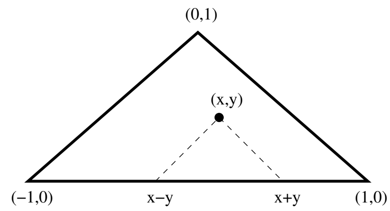
3.1. **Edge-based basis functions.** One part of the high-order basis functions are functions associated with edges. When restricted to an edge, they have to form a basis for $P_0^p(I)$, where $P^p(I)$ denotes the space of polynomials up to order p on the unit interval $I = (-1, 1)$ and the subscript 0 restricts to those polynomials vanishing on the boundary $\{-1, 1\}$. The most commonly used basis functions are the so called integrated Legendre polynomials L_i defined by $L_i(x) = \int_{-1}^{x} P_{i-1}(s)ds$, where the P_i are the Legendre polynomials; see e.g. [1]. Since $\int_{-1}^{1} P_i(s)ds = 0$ for $i \geq 1$, the L_i satisfy zero boundary conditions for $i \geq 2$. The integrated Legendre polynomials satisfy the three-term recurrence

$$\begin{aligned} L_0(x) &= -1, \\ L_1(x) &= x, \\ L_i(x) &= a_i x L_{i-1}(x) + b_i L_{i-2}(x) \qquad \text{for } i \geq 2 \end{aligned}$$

with

$$a_i = \frac{2i-3}{i} \qquad \text{and} \qquad b_i = \frac{3-i}{i}.$$

We note that only the L_i with $2 \leq i \leq p$ form the basis for $P_0^p(I)$. The functions on the open/closed interval I are extended onto the unit triangle T with vertices $(-1, 0)$, $(1, 0)$, $(0, 1)$. For this extension, let $P_0^p(T)$ be the space of polynomials in x and y with maximal total order p and which vanish on the boundary ∂T of T. Note that the boundary ∂T consists of the edges $E_1 = ((-1, 0), (1, 0))$, $E_2 = ((-1, 0), (0, 1))$, and $E_3 = ((1, 0), (0, 1))$ in $\mathbb{R}^2$. The classical extension procedure [3], similar to [9], is the following:

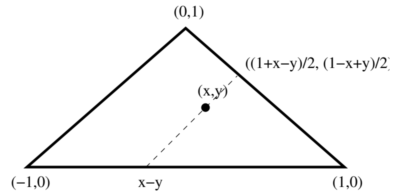


$$\varphi_i^{(1)}(x,y) := \frac{1}{2y}\int_{x-y}^{x+y} L_i(s)\,ds \quad \text{for } y>0.$$

Note that this is an extension of the edge function, in the sense,

$$\varphi_i^{(1)}(x,y) \xrightarrow[y\to 0]{} L_i(x).$$

This extension is bounded as an operator from $H^{1/2}(I) \to H^1(T)$. But, although the polynomials L_i vanish at the boundary of E_1, the extension does not vanish at the two upper edges E_2 and E_3 of the triangle. This can be fixed e.g. by linear interpolation between E_1 and E_2, respectively E_1 and E_3:



Accordingly we define

$$\varphi_i(x,y) := \varphi_i^{(2)}(x,y) - \frac{2y}{1+x+y}\,\varphi_i^{(2)}\left(\frac{x+y-1}{2}, \frac{1+x+y}{2}\right) \tag{4}$$

where

$$\varphi_i^{(2)}(x,y) := \varphi_i^{(1)}(x,y) - \frac{2y}{1-x+y}\,\varphi_i^{(1)}\left(\frac{1+x-y}{2}, \frac{1-x+y}{2}\right). \tag{5}$$

The resulting extension operator preserves the polynomial order and is bounded in the sense that

$$\|\varphi\|_{H^1(T)} \le c\|\varphi\|_{H^{1/2}_{00}(E)}.$$

Moreover, it satisfies zero boundary conditions at the upper two edges E_2 and E_3. Thus, the functions φ_i can be chosen as edge-based shape functions on triangles. Note that the φ_i are considered as shape functions associated to the edge E_1, but shape functions associated to the edge E_2 or E_3 can be immediately obtained from the φ_i by permuting the vertices.

By means of symbolic summation methods we have derived the following relation allowing an efficient computation of the functions φ_i.

Theorem 1. *The functions φ_i as defined in (4) for $i \ge 6$ satisfy the recurrence relation*

$$\varphi_i = a_i x\varphi_{i-1} + (b_i + c_i(x^2-y^2))\varphi_{i-2} + d_i x\varphi_{i-3} + e_i\varphi_{i-4} \tag{6}$$

with the coefficients

$$a_i = \frac{2(2i-3)}{(i+1)}, \qquad b_i = -\frac{(2i-5)(3-10i+2i^2)}{i(i+1)(2i-7)}, \quad c_i = -\frac{(2i-5)(21-20i+4i^2)}{i(i+1)(2i-7)},$$
$$d_i = \frac{2(i-5)(2i-3)}{i(i+1)}, \quad e_i = -\frac{(i-6)(i-5)(2i-3)}{i(i+1)(2i-7)}.$$

The recurrence is started with

$$\begin{aligned}
\varphi_2(x,y) &= 1/2(1+x-y)(1-x-y),\\
\varphi_3(x,y) &= 1/2(1+x-y)(1-x-y)x,\\
\varphi_4(x,y) &= 1/8(1+x-y)(1-x-y)(-1+5x^2-2y+3y^2),\\
\varphi_5(x,y) &= 1/24(1+x-y)(1-x-y)x(-9+21x^2-14y+35y^2).
\end{aligned}$$

Remark. The coefficients a_i to e_i are computed once and for all and are stored in tables. The evaluation of p basis functions φ_i takes just $11p+O(1)$ floating point operations.

3.2. **Discovering and proving Theorem 1.** Using the Sigma package one can find and prove the recurrence (6) as follows. First we transform integrals into sums by starting with the sum representation

$$P_i(x) = (2x)^i \frac{(\frac{1}{2})_i}{i!} \sum_{k=0}^{i} \frac{(-\frac{i}{2})_k(\frac{1-i}{2})_k}{(-i+\frac{1}{2})_k k!}\left(\frac{1}{x}\right)^{2k} \tag{7}$$

(e.g. [1, (6.4.12)]); here we use the standard Pochhammer symbol $(a)_k = a(a+1)\cdot\ldots\cdot(a+k-1)$ for $k>0$, $(a)_0=1$, and $(a)_{-1}=\frac{1}{a-1}$. The representation (7) allows simple term-wise integration and one finds that $\varphi_i^{(1)}$ can be written in the form

$$\varphi_i^{(1)}(x,y) = S(x+y) - S(x-y)$$

where

$$S(Z) = -\sum_{k=0}^{i} \frac{2^{-2k+i-1} Z^{-2k+i+1}\left(-\frac{1}{2}\right)_i (-i)_{2k-1}}{yk!i!\left(\frac{3}{2}-i\right)_k}.$$

Thus, together with (5) and (4), we can write φ_i for $i \geq 2$ as

$$\begin{aligned}
\varphi_i = &-\frac{2^{i-1}y\big((-1)^i(x+y-1)(x+y+3)(-x+y+1)^2+(x-y-3)(x-y+1)(x+y+1)^2\big)\left(-\frac{1}{2}\right)_i}{(x+y+1)^2(x-y-1)^2 i!}A_i\\
&+\frac{(x-3y-1)(x-y)(x+y-1)}{2(x-y-1)^2 y}B_i(x-y) - \frac{(x-y+1)(x+y)(x+3y+1)}{2y(x+y+1)^2}B_i(x+y)
\end{aligned} \tag{8}$$

where the sums A_i, $B_i(x-y)$ and $B_i(x+y)$ are defined by

$$A_i = \sum_{k=0}^{i} \frac{2^{-2k}(-i)_{2k-1}}{k!\left(\frac{3}{2}-i\right)_k} \qquad \text{and} \qquad B_i(Z) = \sum_{k=0}^{i} \frac{2^{i-2k}Z^{i-2k}\left(-\frac{1}{2}\right)_i (-i)_{2k-1}}{i!k!\left(\frac{3}{2}-i\right)_k}.$$

Given this representation, we are ready to apply Sigma.

• We insert the sum A_i in the computer algebra system Mathematica

In[3]:= $\boldsymbol{A = \sum_{k=0}^{i} \frac{2^{-2k}(-i)_{2k-1}}{k!\left(\frac{3}{2}-i\right)_k};}$

and call Sigma to simplify it:

In[4]:= **SigmaReduce[*A*]**

Out[4]= 0

Hence our indefinite summation algorithm yields, for $i \geq 3$,

$$A_i = 0. \tag{9}$$

The proof, resp. proof certificate, of this fact is also delivered automatically by Sigma.

Proof of (9). Let $f(i,k) := \frac{2^{-2k}(-i)_{2k-1}}{k!\left(\frac{3}{2}-i\right)_k}$. The correctness follows from

$$g(i,k+1) - g(i,k) = f(i,k) \tag{10}$$

and the proof certificate given by $g(i,k) = \frac{4k\left(i^2-3i+4k-2\right)}{(i-2)(i-1)i(i+1)} f(i,k)$. Namely, one can conclude that (10) holds for all $i \geq 3$ and all $0 \leq k \leq i$ as follows: Represent $g(i,k+1)$ in terms of $\mathrm{rat}(i,k) f(i,k)$ where $\mathrm{rat}(i,k)$ is a rational function in i and k by using the relation $f(i,k+1) = \frac{2(i-2k)(i-2k+1)}{(k+1)(-2i+2k+1)} f(i,k)$. Then verify (10) by simple polynomial arithmetic. Finally, summing (10) over k gives $A_i = \frac{4^{-i}\left(i^2+i+2\right)(-i)_{2i-1}}{(i^2-i-2)i!\left(\frac{3}{2}-i\right)_i} = 0$ because of $(-i)_{2i-1} = 0$. $\square$

But it should be noted explicitly that for $i = 0, 1, 2$, the sum A_i is not 0. Summarizing, we can neglect the sum expression A_i in φ_i from $i \geq 3$ on.

• Next, we consider the sum $B_i(Z)$. This time we compute a recurrence relation for $B_i(Z)$. We type in

In[5]:= $\boldsymbol{B = \sum_{k=0}^{i} \frac{2^{i-2k} Z^{i-2k}\left(-\frac{1}{2}\right)_i (-i)_{2k-1}}{i!k!\left(\frac{3}{2}-i\right)_k};}$

and run

In[6]:= **recB=GenerateRecurrence[*B*][[1]]**

Out[6]= $\{(i-2)\mathrm{SUM}[i] - (2i+1)Z\,\mathrm{SUM}[i+1] + (i+3)\mathrm{SUM}[i+2] == 0\}$

This means $B_i(Z) = \mathrm{SUM}[i]$ satisfies the recurrence relation in the output Out[6]. Again Sigma delivers automatically a certificate for its correctness.

Proof of Out[6]. Let $f(i,k) := \frac{2^{i-2k}Z^{i-2k}\left(-\frac{1}{2}\right)_i(-i)_{2k-1}}{i!k!\left(\frac{3}{2}-i\right)_k}$. The correctness follows by

$$c_0(i)f(i,k) + c_1(i)f(i+1,k) + c_2(i)f(i+2,k) = g(i,k+1) - g(i,k) \tag{11}$$

and by the proof certificate $c_0(i) = (i-2)$, $c_1(i) = -(2i+1)Z$, $c_2(i) = (i+3)$ and $g(i,k) = -\frac{2(i-2)(2i-2k-1)kZ^2}{(i-2k+2)(i-2k+3)} f(i,k)$. Then by using the relation $f(i,k+1) = \frac{(-i+2k-1)(2k-i)}{2(k+1)(-2i+2k+3)Z^2} f(i,k)$, we can check by polynomial arithmetic that (11) holds for all $i \geq 0$ and $0 \leq k \leq i$. Finally, summing (11) over k and compensating missing terms leads to the recurrence relation in Out[6]. $\square$

Summarizing, $B_i(x-y)$ satisfies for $i \geq 0$ the recurrence

In[7]:= $\text{recB1} = \boldsymbol{(i-2)}\text{SUM}[\boldsymbol{i}] - \boldsymbol{(2i+1)(x-y)}\,\text{SUM}[\boldsymbol{i+1}] + \boldsymbol{(i+3)}\text{SUM}[\boldsymbol{i+2}] == \boldsymbol{0}$

and $B_i(x+y)$ satisfies for $i \geq 0$ the recurrence

In[8]:= $\text{recB2} = \boldsymbol{(i-2)}\text{SUM}[\boldsymbol{i}] - \boldsymbol{(2i+1)(x+y)}\,\text{SUM}[\boldsymbol{i+1}] + \boldsymbol{(i+3)}\text{SUM}[\boldsymbol{i+2}] == \boldsymbol{0}$

To complete the proof of Theorem 1 we use the package GeneratingFunctions to compute a recurrence that is satisfied by both, $B_i(x+y)$ and $B_i(x-y)$.

In[9]:= **RecurrencePlus**[recB1**,** recB2**,** SUM[$\boldsymbol{i}$]]

Out[9]= $$(i-2)(i-1)(2i+5)\text{SUM}[i] - 2(i-1)(2i+1)(2i+5)x\text{SUM}[i+1] \\ + (2i+3)\left(4x^2i^2 - 4y^2i^2 + 2i^2 + 12x^2i - 12y^2i + 6i + 5x^2 - 5y^2 - 5\right)\text{SUM}[i+2] \\ - 2(i+4)(2i+1)(2i+5)x\text{SUM}[i+3] + (i+4)(i+5)(2i+1)\text{SUM}[i+4] == 0$$

Obviously also φ_i is a solution of Out[9] for $i \geq 3$ by (8) and (9). Considering the initial cases $i = 0, 1, 2$, it turns out that only for $i = 0$, our derived recurrence does not hold. The fact that the recurrence from Out[9] is nothing else than (6) completes our proof of Theorem 1.

3.3. **Low energy vertex functions.** The p-dependence of the condition number can be reduced by the use of low energy vertex shape functions. The proposal in [4] is to use vertex shape functions being constant along the level-sets of the standard hat-basis-functions, and minimizing the H^1 norm among this class of functions. This leads to the one-dimensional constrained minimization problem

$$\min_{\substack{v \in P^p(I) \\ v(-1)=0, v(1)=1}} \int_{-1}^{1} (s-1)^{d-1} (v'(s))^2 \, ds, \tag{12}$$

where d is the space dimension, which is $d = 2$ or $d = 3$. This is a strictly convex minimization problem on a finite dimensional space. Thus there exists a unique minimizing polynomial which we call $u_p^d(x)$. To find it we expand v in terms of the Jacobi polynomials $P_i^{(d-2,-1)}$ of order $i = 1, \ldots, p$; see e.g. [1] for their basic properties. Note that Jacobi polynomials $P^{(\alpha,\beta)}$ are defined for parameters $\alpha, \beta > -1$, but, the properties we need are also valid for $\beta = -1$. Jacobi-polynomials can be described recursively by

$$\begin{aligned} P_0^{(\alpha,\beta)}(x) &= 1, \\ P_1^{(\alpha,\beta)}(x) &= 1/2[2(\alpha+1) + (\alpha+\beta+2)(x-1)], \\ P_i^{(\alpha,\beta)}(x) &= a_i P_{i-1}^{(\alpha,\beta)}(x) + b_i P_{i-2}^{(\alpha,\beta)}(x), \qquad \text{for } i \geq 2, \end{aligned}$$

with the coefficients

$$a_i = \frac{(2i+\beta+\alpha-1)(\alpha^2-\beta^2+(2i+\alpha+\beta-2)(2i+\alpha+\beta)x)}{2i(\alpha+\beta+i)(2i+\alpha+\beta-2)}$$

and

$$b_i = -\frac{(i+\alpha-1)(i+\beta-1)(2i+\alpha+\beta)}{i(i+\alpha+\beta)(2i+\alpha+\beta-2)}.$$

By means of the $p \times p$ matrix A defined by

$$A_{i,j} = \int_{-1}^{1} (s-1)^{d-1} (P_i^{(d-2,-1)})'(s) (P_j^{(d-2,-1)})'(s)\, ds,$$

and the vectors $b^0 = (b_1^0, \ldots, b_p^0)$ and $b^1 = (b_1^1, \ldots, b_p^1)$ defined by

$$b_i^0 = P_i^{(d-2,-1)}(-1) \qquad \text{and} \qquad b_i^1 = P_i^{(d-2,-1)}(1),$$

the constrained minimization problem is an algebraic minimization problem, namely

$$\min_{\substack{v\in\mathbb{R}^p \\ b^0\cdot v=0,\, b^1\cdot v=1}} v^T A v.$$

Now, we compute the matrix and vector entries. For the matrix entries $A_{i,j}$ we first use the fact (e.g. [1, (6.4.22)]) that the derivative of a Jacobi polynomial $P_i^{(\alpha,\beta)}$ is given by

$$\frac{d}{dx} P_i^{(\alpha,\beta)}(x) = 1/2(i+\alpha+\beta+1) P_{i-1}^{(\alpha+1,\beta+1)}(x), \qquad i \geq 1,$$

and second that the $P_i^{(\alpha,\beta)}$ are orthogonal w.r.t. the weight function $w_{\alpha,\beta}(x) = (1-x)^\alpha (1+x)^\beta$, i.e.,

$$\int_{-1}^{1} (1-x)^\alpha (1+x)^\beta P_i^{(\alpha,\beta)}(x) P_j^{(\alpha,\beta)}(x)\, dx = \frac{2^{\alpha+\beta+1}}{2i+\alpha+\beta+1} \frac{\Gamma(i+\alpha+1)\Gamma(i+\beta+1)}{i!\Gamma(i+\alpha+\beta+1)} \delta_{i,j}.$$

From this and from our specific choice of parameters $\alpha = d-2,\ \beta = -1$ we obtain that the matrix A is a diagonal matrix with $A_{i,i} = i/2$ in the two dimensional case, and with $A_{i,i} = 2(i+1)^2/(2i+1)$ for $d = 3$.

For the computation of the vectors b^0 and b^1 we observe that $P_0^{(d-2,-1)}(-1) = 1$ and $P_i^{(d-2,-1)}(-1) = 0$ for $d = 2, 3$ and $i \geq 1$. So the first constraint $v(-1) = 0$ is always satisfied. Next we use the identity $P_i^{(\alpha,\beta)}(1) = \binom{i+\alpha}{i}$; see [1]. Therefore the vector $b^1 = (b_1^1, \ldots, b_p^1)$ is given by $b_i^1 = 1$ in the two dimensional and $b_i^1 = i+1$ in the three dimensional case. Now solving the minimization problem for $v = (v_1, \ldots, v_p)$ with the specific values for A and b^1 as given above, results in the functions

$$u_p^2(x) = \left(\sum_{k=1}^{p} \frac{1}{k}\right)^{-1} \sum_{k=1}^{p} \frac{1}{k} P_k^{(0,-1)}(x) \tag{13}$$

in the two dimensional case $d = 2$, and

$$u_p^3(x) = \frac{1}{p(p+2)} \sum_{k=1}^{p} \frac{2k+1}{k+1} P_k^{(1,-1)}(x) \tag{14}$$

for the three-dimensional case $d = 3$. For a fast computation it is sufficient to have a good recursive description for

$$v_p^2(x) := \left(\sum_{k=1}^{p} \frac{1}{k}\right) u_p^2(x) \qquad \text{and} \qquad v_p^3(x) := p(p+2)u_p^3(x),$$

which is stated in the theorem below.

Theorem 2. *The functions v_p^2 and v_p^3 satisfy the recurrence relations*

$$\begin{aligned}
v_1^2(x) &= \frac{x+1}{2},\\
v_2^2(x) &= \frac{3}{8}(x+1)^2,\\
v_3^2(x) &= \frac{1}{24}(x+1)\left(10x^2+5x+7\right),\\
v_p^2(x) &= \frac{(2p-1)(-1+3x+p^2(1+2x)-p(1+5x))}{p^2(2p-3)} v_{p-1}^2(x)\\
&\quad - \frac{(1+x-3p(1+x)+p^2(1+2x))}{p^2} v_{p-2}^2(x) + \frac{(p-2)^2(2p-1)}{p^2(2p-3)} v_{p-3}^2(x),
\end{aligned}$$

and

$$\begin{aligned}
v_1^3(x) &= \frac{3(1+x)}{2},\\
v_2^3(x) &= \frac{1}{2}(1+x)(3+5x),\\
v_p^3(x) &= \frac{(x(4p^2-1)-1)}{(p+1)(2p-1)} v_{p-1}^3(x) - \frac{(p-1)(2p+1)}{(p+1)(2p-1)} v_{p-2}^3(x) + \frac{(2p+1)(1+x)}{(p+1)},
\end{aligned}$$

respectively.

3.4. **Discovering and proving Theorem 2.** We start with the sum $v_p^3(x)$ by typing in

In[10]:= $\mathbf{v3} = \sum_{k=1}^{p} \frac{2k+1}{k+1} P1[k];$

Moreover, we insert the defining recurrence relation for $P1[k] := P_k^{(1,-1)}(x)$,

In[11]:= $\mathbf{recP1} = k(k+2)\mathrm{P1}[k] - (k+1)(2k+3)x\mathrm{P1}[k+1] + (k+1)(k+2)\mathrm{P1}[k+2] == 0;$

see [1]. The first values are

In[12]:= $P1[1] = x+1; \quad P1[2] = \frac{3}{2}x(x+1);$

Next, we apply our indefinite summation algorithm and obtain a closed form for $v_p^3(x)$:

In[13]:= $\mathbf{SigmaReduce}[\mathbf{v3}, \mathbf{recP1}, P1[k]]$

Out[13]= $-\frac{x+1}{x-1} - \frac{p\,\mathrm{P1}[p]}{(p+1)(x-1)} + \frac{\mathrm{P1}[p+1]}{x-1}$

Proof. Let $f(p,k) := \frac{2k+1}{k+1}P1[k]$. The correctness follows from

$$g(p,k+1) - g(p,k) = f(p,k) \tag{15}$$

and the proof certificate given by $g(p,k) = \frac{(-2xk+k-x+1)\mathrm{P1}[k]+(k+1)\mathrm{P1}[k+1]}{(k+1)(x-1)}$. Namely, one can conclude that (15) holds for all $1 \le k \le p$ and all $p \ge 0$ as follows: Express $g(p,k+1)$ in terms of $P1[p]$ and $P1[p+1]$ by using the recurrence given in In[11]. Then verify (15) by polynomial arithmetic. Finally, summing (15) over k from 0 to p gives Out[13]; here we used the initial values from Out[12]. □

Summarizing, we have discovered and proven that

$$v_p^3(x) = \sum_{k=1}^{p} \frac{2k+1}{k+1} P_k^{(1,-1)}(x) = -\frac{x+1}{x-1} - \frac{pP_p^{(1,-1)}(x)}{(p+1)(x-1)} + \frac{P_{p+1}^{(1,-1)}(x)}{x-1} \tag{16}$$

for all $p \ge 1$. Note that with this result we can easily obtain a recurrence for $v_p^3(x)$ by first inserting recurrence relations for $-\frac{p\,\mathrm{P1}[p]}{(p+1)(x-1)}$, $\frac{\mathrm{P1}[p+1]}{x-1}$ and $-\frac{x+1}{x-1}$ and then adding the recurrence relations like in In[9]. But, since the resulting recurrence is rather big (a recurrence of order 4), we follow another strategy.

We insert into the sum $v3$ the factor $\frac{(e-k+p)!}{(-k+p)!}$ where e is some additional slack parameter. Note that this factor reduces to 1, if we send e to 0.

In[14]:= $\mathbf{v3e} = \sum_{k=1}^{p} \frac{(e-k+p)!}{(-k+p)!}\frac{(2k+1)}{(k+1)}\mathbf{P1[k]}$

Then we apply our definite summation algorithm and obtain a recurrence relation for $\mathrm{v3e} = \mathrm{SUM}[p]$.

In[15]:= **GenerateRecurrence[v3e, p, {recP1, P1[k]}]**

Out[15]=
$$\begin{aligned}
&(-e-p-1)(e+2p+6)\mathrm{SUM}[p]\\
&+\left(2xe^2+(6xp+p+15x+3)e+2\left((2x+1)p^2+(9x+5)p+9x+5\right)\right)\mathrm{SUM}[p+1]\\
&+\left(-e^2-(7x+p(2x+3)+8)e-2\left((2x+1)p^2+(11x+5)p+14x+5\right)\right)\mathrm{SUM}[p+2]\\
&+(p+4)(e+2p+4)\mathrm{SUM}[p+3]\\
&== \frac{(e+p)(e+p+1)\left(3e^2+6(p+2)e+4p^2+18p+20\right)(x+1)(e+p-1)!}{p\left(p^2+3p+2\right)(p-1)!}
\end{aligned}$$

Proof of Out[15]. Let $f(p,e,k) := \frac{(e-k+p)!}{(-k+p)!)}\frac{(2k+1)}{(k+1)}P1[k]$. The correctness follows by

$$c_0(e,p)f(e,p,k) + \cdots + c_3(e,p)f(e,p+3,k) = g(e,p,k+1) - g(e,p,k) \tag{17}$$

and the proof certificate given by

$$\begin{aligned}
c_0(e,p) &= -(e+p+1)(e+2p+6),\\
c_1(e,p) &= 2xe^2+(6xp+p+15x+3)e+2((2x+1)p^2+(9x+5)p+9x+5),\\
c_2(e,p) &= -e^2-(7x+p(2x+3)+8)e-2((2x+1)p^2+(11x+5)p+14x+5),\\
c_3(e,p) &= (p+4)(e+2p+4)
\end{aligned}$$

and

$$g(p,k) = \frac{(e-k+p+1)(e-k+p)!\big[g_0(p,k)P1[k] + g_1(p,k)P1[k+1]\big]}{(p-k)!(k+1)(k-p-3)(k-p-2)(k-p-1)}$$

where

$$\begin{aligned} g_0(p,k) &= (2k^2+3k+1)e^3 + (2k+1)((2x-1)k^2 \\ &\quad + (p(3-2x)-3x+5)k - 3p(x-1) - 9x + 6)e^2 + 2(2(p+2)(2x-1)k^3 \\ &\quad - ((4x-2)p^2 + 3(4x-1)p + 8x + 3)k^2 - (p+2)(21x + p(8x-5) - 10)k - 3p^2(x-1) \\ &\quad - 15p(x-1) - 18x + 19)e - 2(2p+5)(k^2 - (2p+5)k + p^2 + 5p + 6)(x + k(2x-1) - 1) \end{aligned}$$

and

$$g_1(p,k) = (k+1)(p-k+3)((2k+3)e^2 + 2(2k+3)(p+2)e - 2(k-p-2)(2p+5)).$$

The correctness of (17) can be verified for all $0 \leq k \leq p$ and for all $p \geq 0$ in the same way as for (15). Hence summing (17) and taking into account the initial values In[12] produces Out[15]. □

Setting $e = 0$ in our computed recurrence gives a recurrence relation for our desired $v_p^3(x) = \mathrm{SUM}[p]$:

In[16]:= $\mathbf{rec = rec/.e \to 0}$

Out[16]= $-(p+1)(p+3)\mathrm{SUM}[p] + ((2x+1)p^2 + (9x+5)p + 9x + 5)\mathrm{SUM}[p+1]$
$+ (-2xp^2 - p^2 - 11xp - 5p - 14x - 5)\mathrm{SUM}[p+2] + (p+2)(p+4)\mathrm{SUM}[p+3] == (2p+5)(x+1)$

Remarkably, we can simplify this recurrence further by another application of Sigma. To this end, we insert the first initial values $v_p^3(x)$ for $p = 1,2,3$

In[17]:= $\mathbf{eval = \{\frac{3}{2}(x+1), \frac{1}{2}(x+1)(5x+3), \frac{5}{8}(x+1)\left(7x^2+4x+1\right)\};}$

Then the following procedure call produces a simpler recurrence, i.e.,

In[18]:= **ReduceRecurrence[rec, SUM[p], 1, eval]**

Out[18]= $(-p-1)(2p+5)\mathrm{SUM}[p] + \left(\left(4p^2+16p+15\right)x - 1\right)\mathrm{SUM}[p+1]$
$- (p+3)(2p+3)\mathrm{SUM}[p+2] == (-2p-3)(2p+5)(x+1)$

Proof of Out[18]. The correctness follows by

$$g(p+1) - g(p) = 0 \tag{18}$$

with the proof certificate

$$g(p) := \frac{(4p^2-17)(x+1) - (p+1)(2p+5)\mathrm{SUM}[p] + (4xp^2+16xp+15x-1)\mathrm{SUM}[p+1] - (p+3)(2p+3)\mathrm{SUM}[p+2]}{(p+2)(x+1)}.$$

From this one can conclude that (18) holds for all sequences SUM[p] that satisfy the recurrence from Out[16]: Express $g(p+1)$ in terms of SUM[p], SUM[$p+1$] and SUM[$p+2$] by using the recurrence given in Out[16]. Afterwards verify (18) by polynomial arithmetic. Owing to (18), it follows that $g(p)$ does not depend anymore on p. Plugging the initial values In[17] into g gives $g = -16$. This is nothing else than Out[18]. □

Alternative correctness proof. Replace SUM[$p+i$] in Out[18] with $\sum_{k=1}^{p}\frac{2k+1}{k+1}P1[k]+\sum_{k=1}^{i}\frac{2(p+k)+1}{(p+k)+1}P1[k]$ for $i=0,1,2$; here we consider $\sum_{k=1}^{p}\frac{2k+1}{k+1}P1[k]$ symbolically, i.e., do not apply any simplification. Then by polynomial arithmetic we arrive at

$$\sum_{k=1}^{p}\frac{(2k+1)\mathrm{P1}[k]}{k+1}=\frac{-(2xp-p+3x-2)\mathrm{P1}[p+1]-(p+2)(x-\mathrm{P1}[p+2]+1)}{(p+2)(x-1)}. \tag{19}$$

Note that Out[18] is correct if (19) is correct. Representing P1[$p+2$] in terms of P1[p] and P1[$p+1$] by using In[11] gives (16); but (16) has been proven. □

Finally, we apply exactly the same summation tools to the sum $v_p^2(x)$ where $P2[k]=P_k^{(0,-1)}(x)$ fulfills the following recurrence relation; see [1].

In[19]:= $\mathbf{recP2 = k(2k+3)P2[k]+\left(1-\left(4k^2+8k+3\right)x\right)P2[k+1]+(k+2)(2k+1)P2[k+2]==0;}$

Note that this time we fail to find a closed form evaluation of the type (16). Therefore we apply our definite summation tools. First, we insert the sum

In[20]:= $\mathbf{v2e}=\sum_{k=1}^{p}\frac{(e-k+p)!}{k(p-k)!}\mathbf{P2}[k]$

which is $v_p^2(x)$ after sending e to 0. Using Sigma we get the recurrence relation

In[21]:= $\mathbf{rec = GenerateRecurrence[v2e}, p, \{\mathbf{recP2, P2}[k]\}]/.e\to 0$

Out[21]= $(p+3)(p+1)^2\mathrm{SUM}[p]+(-2(x+1)p^3-(13x+12)p^2-(27x+22)p-18x-13)\mathrm{SUM}[p+1]$
$+(2p+5)((2x+1)p^2+5(2x+1)p+12x+5)\mathrm{SUM}[p+2]$
$+(-2(x+1)p^3-(17x+18)p^2-(47x+52)p-42x-47)\mathrm{SUM}[p+3]+(p+2)(p+4)^2\mathrm{SUM}[p+4]==0$

for SUM[p] $=v_p^2(x)$. Finally, we can simplify the recurrence relation by using the first initial values of $v_p^2(x)$ with $p=1,2,3,4$

In[22]:= $\mathbf{eval}=\left\{\frac{x+1}{2},\frac{3}{8}(x+1)^2,\frac{1}{24}(x+1)\left(10x^2+5x+7\right),\frac{5}{192}(x+1)^2\left(21x^2-14x+13\right)\right\}$

and by calling the procedure

In[23]:= $\mathbf{ReduceRecurrence[rec, SUM}[p]\mathbf{, eval]}$

Out[23]= $(2p+5)(p+1)^2\mathrm{SUM}[p]-(2p+3)((2x+1)p^2+(9x+3)p+10x+1)\mathrm{SUM}[p+1]$
$+(2p+5)((2x+1)p^2+(7x+5)p+6x+5)\mathrm{SUM}[p+2]-(p+3)^2(2p+3)\mathrm{SUM}[p+3]==0$

Proof of Out[21]. Replace SUM[$p+i$] in Out[21] with $\sum_{k=1}^{p}\frac{1}{k}P2[k]+\sum_{k=1}^{i}\frac{1}{p+k}P2[k]$ for $i=0,1,2,3$. By simple polynomial arithmetic the correctness follows. □

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