Computer algebra and Umbral Calculus

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Abstract

Rota's Umbral Calculus uses sequences of Sheffer polynomials to count certain combinatorial objects. We review this theory and some of its generalizations in light of our computer implementation (Maple V.3). A Mathematica version of this package is being developed in parallel.

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1. Introduction

Umbral Calculus is the study of the analogies between various polynomial sequences and the powers sequence \( x^n \). For example, \( x^n \) has many parallels with the lower factorial sequence \( (x)_n = x(x-1) \cdots (x-n+1) \):

- The forward difference operator \( A: p(x) \rightarrow p(x + 1) - p(x) \) plays a defining role with respect to \( (x)_n \), analogous to that played by the derivative \( d \) with respect to \( x^n \).
- Taylor's theorem is analogous to Newton's theorem.
- The binomial theorem for \( (x+y)^n \) is replaced by Vandermonde's identity for \( (x+y)_n \).

Although Umbral Calculus dates back to the 18th century, it was only put on a rigorous foundation by Gian-Carlo Rota and his collaborators [8, 16] in the 1970s. We now characterize each polynomial sequence under study by one or more polynomial operators associated with it. The duality between operators and polynomials is the key tool to deriving Umbral Calculus results.

Umbral Calculus has many applications in enumerative combinatorics. The powers \( x^n \) count all functions from an \( n \)-element set to an \( x \)-element set, while the lower
factorials \((x)_n\) count injections. Similarly, given any species of combinatorial structures (or quasi-species), let \(p_n(x)\) be the number of functions from an \(n\)-element set to an \(x\)-element set enriched by this species. A function is enriched by associating a (weighted) structure with each of its fibers. The resulting sequence of polynomials \((p_n)_{n \in \mathbb{N}}\) is said to be of binomial type since it obeys the 'binomial' identity

\[
p_n(x + y) = \sum_{k=0}^{n} \binom{n}{k} p_k(x)p_{n-k}(y).
\]

For example, given the species of rooted forests, the enriched functions are called\textit{reluctant functions} and are enumerated by the Abel polynomials \(A_n(x) = x(x + n)^{n-1}\). Other applications of the Umbral Calculus include lattice path counting [10,11,19].

Our Maple package provides a number of different tools by which to enter operators. These operators can then be manipulated in many different ways. In particular, the polynomial sequences associated with them can be explicitly calculated.

This package has already aided us in our research [4]; we hope that it will help you too.

We expect to release a Mathematica version of this package in the near future.

2. Basic results of Umbral Calculus

In this section we give an overview of the main results from Umbral Calculus. The seminal paper [16] still makes excellent reading; its precursor [8] contains a preliminary form of the theory and contains more combinatorial applications. More recent expositions can be found in [13] and [15]. An electronic survey [3] of the Umbral Calculus with an extensive bibliography is available over the World Wide Web.

The Umbral Calculus is based on operators on the vector space of polynomials with coefficients in some field of characteristic zero. A linear operator is said to be \textit{shift-invariant} if it commutes with the shift operators \(E^a : p(x) \rightarrow p(x + a)\). A \textit{delta operator} is a shift-invariant operator \(Q\) such that \(Qx\) is a non-zero constant. It can be shown that delta operators reduce the degree of polynomials by one [16, Proposition 3, p. 688]. The \textit{basic sequence} for a delta operator \(Q\) is the unique sequence \((P_n)_{n \in \mathbb{N}}\) of polynomials with the properties \(Qp_n = np_{n-1}\), \(p_0 = 0\), and \(p_n(0) = 0\) for \(n \geq 1\). A fundamental theorem of Umbral Calculus [16, Theorem 1, p. 689] says that each basic sequence is of binomial type, i.e., it satisfies the binomial-like identity

\[
p_n(x + y) = \sum_{k=0}^{n} \binom{n}{k} p_k(x)p_{n-k}(y).
\]

Conversely, for each sequence \((p_n)_{n \in \mathbb{N}}\) of binomial type, \(^1\) the unique linear operator \(Q\) defined by \(Qp_n = np_{n-1}\) turns out to be shift-invariant [16, Theorem 1, p. 689].

\(^1\)We assume here and in the sequel that all polynomial sequences \((p_n)\) are such that \(\deg p_n = n\).
Many Umbral Calculus identities follow from the following lemma (cf. [9,2]).

**Lemma 1.** Let \((p_n)_{n \in \mathbb{N}}\) and \((q_n)_{n \in \mathbb{N}}\) be two polynomial sequences. If there exists a delta operator \(Q\) and scalars \((v_n)_{n \in \mathbb{N}}\) such that

- \(p_n(v_n) = q_n(v_n)\) for all \(n\),
- \(Qp_n = np_{n-1}\) for \(n = 1, 2, \ldots\),
- \(Qq_n = nq_{n-1}\) for \(n = 1, 2, \ldots\),

then \(p_n = q_n\) for all \(n\).

**Proof.** Follows by induction, since the kernel of a delta operator consists of constants only. \(\square\)

The following sequences of polynomials are of binomial type.

**Powers of \(x\):** Their delta operator is the derivative operator. They count the number of maps from an \(n\)-element set to an \(x\)-element set.

**Lower factorials:** Their delta operator is the forward difference operator. They count the number of injections from an \(n\)-element set to an \(x\)-element set.

**Upper factorials:** Their delta operator is the backward difference operator. They count the number of dispositions. A disposition is a function with a linear order on each fiber. It may be thought of as an assignment of flags to flagpoles in which the flags on any given flagpole are placed in a certain order.

**Abel polynomials:** Their delta operator is \(D \circ E^a\), where \(D\) is the derivative operator and \(E^a\) is the shift-operator. They count the enriched functions of the species of rooted forests.

**Laguerre polynomials:** Their delta operator maps \(p \mapsto \int_0^\infty e^{-t} p(x + t) \, dt\). These polynomials count functions from an \(n\)-element set to an \(x\)-element set enriched with an assembly (or collection) of linear orders on each fiber. Such an enriched function may be thought of as assignment of coins to boxes where the coins can be arranged into a number of piles within each box.

**Mittag–Leffler polynomials:** These polynomials count permutations without cycles of even length. Their generating function is \(\sum_n M_n(x) z^n = ((1 + z)/(1 - z))^\alpha\), which shows that they are of binomial type.

A larger class of polynomial sequences are the Sheffer sequences, i.e., sequences of polynomials \((s_n)_{n \in \mathbb{N}}\) such that \(s_0\) is a non-zero constant and there is delta operator \(Q\) with \(Qs_n = ns_{n-1}\). Sheffer sequences can be shown to be the image under an invertible shift-invariant operator of a basic sequence [16, Proposition 1, p. 698]). The following useful formulas hold for shift-invariant operators and Sheffer sequences (and a fortiori for polynomials of binomial type):

\[
T = \sum_{k=0}^{\infty} (Ts_k)(0)AQ^k, \quad (2)
\]

\[
p = \sum_{k=0}^{\infty} (Qp)(0)s_k, \quad (3)
\]
where \( T \) is an arbitrary shift-invariant operator, \( p \) is an arbitrary polynomial, \((s_n)_{n \in \mathbb{N}}\) is a Sheffer sequence for a delta operator \( Q \) with basic set \((q_n)_{n \in \mathbb{N}}\), and \( A \) is the invertible shift-invariant operator such that \( AQ_n = s_n \).

Given a delta operator \( Q \), its basic sequence \((q_n)_{n \in \mathbb{N}}\) can be recovered by the Transfer Formula [16, Theorem 4, p. 695]

\[
p_n(x) = Q' U^{-n-1} x^n,
\]

(where \( Q' := Qx - xQ \) is the Pincherle derivative of \( Q \) and \( U \) is the unique linear operator such that \( Q = UD \)) or one of its variants, e.g. the Rodrigues Formula [16, Theorem 4, p. 695]:

\[
p_n(x) = x(Q')^{-1} p_{n-1}(x).
\]

The name Umbral Calculus comes from the concept of umbral composition. This was a mystifying operation (see, e.g., [5]) until Rota identified this operation as the linear operator that maps \( x^n \) to \( p_n \), where \((p_n)_{n \in \mathbb{N}}\) is of binomial type (such operators are called umbral operators). The set of Sheffer sequences forms an Abelian group when endowed with umbral composition as group operation.

**Proposition 2** (Di Bucchianico [2]). The only shift-invariant umbral operator is the identity operator.

**Proof.** Let \( T \) be a shift-invariant operator with \( Tx^n = p_n \) and let \( Q \) be the delta operator of \((p_n)_{n \in \mathbb{N}}\). Since \( Dp^n = DTx^n = TDx^n = nTx^n = 1 = np_{n-1}, \) \( p_0 = 1 \) and \( p_n(0) = 0 \) for \( n \geq 1 \), it follows from Lemma 1 that \( n - x^n \). Hence, \( T = I \). \( \Box \)

3. Polynomial operators

In this section we describe our computer algebra package.

Polynomial operators (shift-invariant or not) can be specified within the package in several convenient manners:

* Explicitly by their action on polynomials. For example, the shift operator is defined \(<\text{subs}(x = x+a, p) \mid p>\) using the 'angle-bracket' notation for functional operators.

Similarly, the Bernoulli operator \( p(x) \rightarrow \int_x^{x+1} p(t) dt \) is defined \(<\text{int}(\text{subs}(x = t, p), t = x..(x+1)) \mid p \mid t>\).

* As an analytic function of the derivative. By the expansion formula (2), any shift-invariant operator can be expanded as a formal power series in \( d \) where \( d \) is a special reserved symbol representing the derivative. For example, the shift operator is defined \( \exp(ad) \).

* Abstractly as an unspecified function of \( d \). For example, \( f(d) \) or \( f(d,x) \) in the case of a nonshift-invariant operator [7].
Using the powseries package. If the coefficients of the formal power series given by the expansion theorem are all known, then use powcreate. For example, powseries [powcreate] (f(n) = a^n/n!);

As a series. If only finitely many terms are known, then use series. For example, series(1 + a + d + a^2 + d^2 + a^2 + d^2 + c + d + a^3, d, 3);

Operators can be converted easily from one form to another with convert. A delta operator Q is a shift-invariant operator such that Q x is a nonzero constant. An abstract operator is assumed to be invertible unless indicated otherwise. (For example, Q := d*f(d); or Q := f(d); f(0) := 0;)

Using the expansion formula (2), shift-invariant operators can be expanded with oe as a formal power series in an arbitrary delta operator.

\[
> \text{oe}(d, \text{delta}, 3);
\]

\[
\exp(d) - 1 - 1/2 (\exp(d) - 1)^2 + O((\exp(d) - 1)^3)
\]

Such operator expansions are practical for numerical calculations. For example, expanding the Bernoulli operator into powers of the forward difference operator delta yields the classical Newton–Cotes formula of numerical integration [8, p. 186].

Our package also allows the expansion of linear operators which are not shift-invariant. We use the following expansion formula given without proof in [7].

**Theorem 3.** Let B be a linear operator mapping polynomials to polynomials such that \( \deg Bp = \deg p - 1 \) and let \((b_n)_{n \in \mathbb{N}}\) be the unique sequence of polynomials with the properties \( Bb_n = nb_{n-1} \), \( b_0 = 0 \), and \( b_n(0) = 0 \) for \( n \geq 1 \). Any linear operator T mapping polynomials to polynomials admits the following expansion in powers of B:

\[
T = \sum_{k=0}^{\infty} a_k(X) B^k,
\]

where X is the multiplication by x operator, and the polynomials \( a_k \) are given by the generating function

\[
\sum_{k=0}^{\infty} a_k(x) t^k = \frac{Bb(x, t)}{b(x, t)},
\]

and \( b(x, t) = \sum_{n=0}^{\infty} b_n(x) t^n/n! \) denotes the generating function of \((b_n)_{n \in \mathbb{N}}\).

**Proof.** Apply both sides of Eq. (4) to the basis \( b_k(x) \), or equivalently to its generating function \( b(x, t) \). The left-hand side gives \( Bb(x, t) \) while the right-hand side gives

\[
\sum_{k} a_k(X) B^k b(x, t) = \sum_{k} a_k(x) t^k b(x, t)
\]

\[
= b(x, t)^{-1} (Tb(x, t)) b(x, t)
\]

\[
= Tb(x, t). \quad \Box
\]
For example, if $B = D$ and $T$ is the operator $T: p(x) \rightarrow \int_0^x p(t) \, dt$, then the expansion
\[
\text{convert}(T, \text{function}, 5, x) \text{ or } \text{convert}(T, \text{powseries}, x)
\]
of $T$ in terms of multiplication by $x$ and the derivative $d$ gives an elementary proof of Bourbaki's method of asymptotic integration [1, Sections 3.5 and 3.6].

Operators can be applied to polynomials with $dp$ by specifying the free variable of the polynomial:

\[
> \text{dp}(\text{delta}, x^3, x);
\]

\[
3x^2 + 3x + 1
\]

In case the degree of the polynomial is not explicitly given, the program will calculate the $\text{Order}$ most significant terms of the answer. ($\text{Order}$ is a system variable whose default value is 6.)

\[
> \text{dp}(\text{delta}, x^n, x);
\]

\[
nx^{(n-1)} + \frac{1}{2} n(n-1) x^{(n-2)} + \frac{1}{6} n(n-1)(n-2)x^{(n-3)}
+ \frac{1}{24} n(n-1)(n-2)(n-3)x^{(n-4)}
+ \frac{1}{120} n(n-1)(n-2)(n-3)(n-4) x^{(n-5)} + O(x^{(n-6)})
\]

4. Polynomial sequences

Given the necessary operators, the program can calculate polynomials of binomial type (bfo), Sheffer sequences (sfo), Steffensen sequences (steff), and cross-sequences (cseq) (see [16, Sections 5 and 8]). For example, the sequence of binomial type $bfo(p(d), x, n)$ associated with a delta operator $p(d)$ is defined by the conditions

\[
\text{dp}(p(d), bfo(p(d), x, n)) = n \cdot bfo(p(d), x, n) \text{ for } n > 0
\]
\[
bfo(p(d), 0, n) = 0 \text{ for } n > 0
\]
\[
bfo(p(d), x, 0) = 1
\]

or equivalently by its exponential generating function $\exp(q(x)t)$ where $q$ is the compositional inverse of $p$. Note that $q(t)$ is the generating function of the associated species, where $bfo(p(d), x, n)$ enumerates the number of functions from an $n$-element set to an $x$-element set with a (weighted) S-structure enriching each fiber.

Taking the singleton species $S = X$, the lower factorials form the basic sequence of binomial type for the forward difference operator $\Delta$.

\[
> \text{factor}(\text{bfo}(\text{delta}, x, 4));
\]

\[
x(x - 1)(x - 2)(x - 3)
\]

If the degree is not explicitly given, then only the most significant terms will be computed.
Several functions in the package do further operations on polynomial sequences. Arbitrary polynomials can be expressed in terms of such sequences (polynomialExpansion, shefferExpansion, basicExpansion). For example,

```plaintext
> p := randpoly(x);
p := 79x^5 + 56x^4 + 49x^3 + 63x^2 + 57x - 59
> be(delta, p, x);
- 59 bfo(exp(d) - 1, x, 0) + 304 bfo(exp(d) - 1, x, 1)
+ 1787 bfo(exp(d) - 1, x, 2) + 2360 bfo(exp(d) - 1, x, 3)
+ 846 bfo(exp(d) - 1, x, 4) + 79 bfo(exp(d) - 1, x, 5)
```

Connection constants can be determined between arbitrary polynomial sequences. For example, the Stirling numbers are given by `cc(topseq(powerx(5, x), x), topseq(lower(5, x), x))` where `powerx(n, x)` is `x^n` and `lower(n, x)` is `(x)_n`. Other features include umbral composition (uc), and umbral inversion (ui).

### 5. Generalizations

Several authors (e.g., [13,18]) have generalized the umbral calculus by considering not only sequences of binomial type with generating function `exp(q(x)t)` but also those whose generating function is `\Phi(g(x)t)` where `\Phi(t) = \sum_{n=0}^{\infty} t^n/[n]!` and `[n]!` denotes the generalized factorial `[n]! = a(1)a(2)\cdots a(n)`. Most of the functions in the umbral calculus package allow an optional argument `a` which is either left undefined, or defines the coefficients used by the 'generalized derivative'. Thus,

```plaintext
> dp(d, x^5, x, proc(n) I end);
x^2
```

The following possible choices for `a` are predefined.

<table>
<thead>
<tr>
<th>Umbral Calculus</th>
<th>dp(d, p, x, a)</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Classical [8,16]</td>
<td>( \frac{dp(x)}{dx} )</td>
<td>Classical(n) = n</td>
</tr>
<tr>
<td>q-Umbral Calculus [13,14]</td>
<td>( \frac{p(qx) - p(x)}{(q - 1)x} )</td>
<td>Gaussian(n) = ( \frac{q^n - 1}{q - 1} )</td>
</tr>
<tr>
<td>Divided difference [6,17]</td>
<td>( \frac{p(x) - p(0)}{x} )</td>
<td>Divided(n) = 1</td>
</tr>
<tr>
<td>Hyperbolic [4]</td>
<td>( \left( \frac{d}{dy/\sqrt{x}} \right)^2 p(x) )</td>
<td>Hyperbolic(n) = ( 2n \times (2n - 1) )</td>
</tr>
</tbody>
</table>
Generalizations of the Umbral Calculus to several variables [12,19] are supported. Most functions included in the package have an alternate syntax for use in multivariate umbral calculi. In particular, \( d[i] \) represents the partial derivative with respect to the \( i \)th variable. Instead of a single delta operator, a collection of operators are required to define a sequence of binomial type. This generalization is completely compatible with the above generalization.

References