As an experimental mathematician, my research topics involve computer software and algorithms, where computation is used to investigate mathematical objects and identify properties and patterns. My broaden research interests include Number Theory, Combinatorics, Differential Geometry, and Quantum Computing. Primarily, I study certain numbers, sequences, polynomials, special functions, combinatorial identities, geometric structures, and quantum algorithms, and I focus on their properties that computer algorithms can (in-)directly guide or help to prove. Unlike numerical analysts, who simulate and approximate with models, I pursue analytic and accurate expression and solutions, instead of approximations. More precisely, I mainly work on the following topics.

1 Special Functions and Polynomials in Number Theory and Combinatorics.

This is my main research area, and I focus on special functions and polynomials that are either important, or have deep connections with other fields of mathematics. For instance, Bernoulli and Euler polynomials (e.g., [26, Chpt. 24]) are my favorite objects, and my main tool is the *Bernoulli and Euler symbols*, denoted by $\mathcal{B}$ and $\mathcal{E}$, respectively. Each of the two symbols satisfies a simple evaluation rule: $\mathcal{B}^n = B_n$ and $\mathcal{E}^n = E_n/2$, where B_n and E_n are *Bernoulli and Euler numbers.* Originally, both $\mathcal{B}$ and $\mathcal{E}$ arise from the traditional umbral calculus (see, e.g., [28]). Meanwhile, recent results interpret them as certain random variables. More specifically, by letting, for $t \in \mathbb{R}$,

$$p_B(t) := \pi \text{sech}^2(\pi t)/2 \quad \text{and} \quad p_E(t) := \text{sech}(\pi t),$$

we define two random variables L_B and L_E with density functions p_B and p_E, respectively. Then, with $i^2 = -1$, we have

$$\mathcal{B} = iL_B - 1/2 \quad \text{and} \quad \mathcal{E} = iL_E - 1/2. \tag{1}$$

Note that, (1) implies the evaluation rules are exactly taking the expectation. This probabilistic interpretation widely not only provides a rigorous background, also largely extends the application of symbolic computations.

1.1 Extensions

Beyond traditional umbral symbol that only expresses Bernoulli and Euler polynomials, by viewing them as random variables, we could define

$$\mathcal{B}^{(p)} := \mathcal{B}_1 + \cdots + \mathcal{B}_p \quad \text{and} \quad \mathcal{E}^{(p)} := \mathcal{E}_1 + \cdots + \mathcal{E}_p.$$

Here, $(\mathcal{B}_i)_{i=1}^p$ is a sequence of independent and identically distributed (i. i. d.) random variables with each $\mathcal{B}_i$ having the same distribution as $\mathcal{B}$, denoted as $\mathcal{B}_i \sim \mathcal{B}$. Similarly define a sequence of i. i. d. random variables $(\mathcal{E}_i)_{i=1}^p$ with $\mathcal{E}_i \sim \mathcal{E}$. Then, extensions on higher-order polynomials and Bernoulli-Barnes ones are expressed, symbolically as follows.

- Bernoulli and Euler polynomials of order p, $B_n^{(p)}(x)$ and $E_n^{(p)}(x)$:

$$B_n^{(p)}(x) = \mathbb{E}\left[\left(x + \mathcal{B}^{(p)}\right)^n\right] \quad \text{and} \quad E_n^{(p)}(x) = \mathbb{E}\left[\left(x + \mathcal{E}^{(p)}\right)^n\right];$$

- Bernoulli-Barnes polynomials $B_n(\mathbf{a}; x)$, with $\mathbf{a} = (a_1, \ldots, a_k)$ and $a_l \neq 0$:

$$B_n(\mathbf{a}; x) = \mathbb{E}\left[\frac{(x + a_1\mathcal{B}_1 + \cdots + a_k\mathcal{B}_k)^n}{a_1 a_2 \cdots a_k}\right],$$

  where $\boldsymbol{\mathcal{B}} = (\mathcal{B}_1, \ldots, \mathcal{B}_k)$ and $\mathbf{a} \cdot \boldsymbol{\mathcal{B}} = \sum_{l=1}^k a_l \mathcal{B}_l$.

Results based on symbolic expressions extends traditional ones. For the Bernoulli-Barnes polynomials $B_n(\mathbf{a}; x)$, Bayad and Beck [2] obtained several properties such as the difference formula

$$(-1)^m B_m(\mathbf{a}; -x) - B_m(\mathbf{a}; x) = m! \sum_{j=0}^{n-1} \sum_{|J|=j} \frac{B_{m-n+j}(\mathbf{a}_J; x)}{(m-n+j)!}; \tag{2}$$

and the self-duality of sequence $\left((-1/A)^n B_n(\mathbf{a}; 0)\right)_{n=0}^\infty$, where $A := a_1 + \cdots + a_n \neq 0$, and the symmetry formula. In [18], based on the symbolic expression, we show that, for polynomial P,

$$P(x - \mathbf{a} \cdot \boldsymbol{\mathcal{B}}) = \sum_{j=0}^n \sum_{|J|=j} |a|_{J^*} P^{(n-j)}(x + (\mathbf{a} \cdot \boldsymbol{\mathcal{B}})_J),$$

where $J \subset [n] := \{1, \ldots, n\}$ and $J^* = [n] \backslash J$, which, by taking $P(x) = x^m/(|\mathbf{a}|\, m!)$ gives (2). Namely, the symbolic expression of $B_n(\mathbf{a}; x)$ gives a more general result. Also, for the self-duality of $\left((-1/A)^n B_n(\mathbf{a}; 0)\right)_{n=0}^{\infty}$, we gave a direct proof that Bayad and Beck asked for.

1.2 Multiple zeta value at non-positive integers

The multiple zeta function

$$\zeta_r(n_1, \ldots, n_r) = \sum_{k_1, \ldots, k_r > 0} \frac{1}{k_1^{n_1}(k_1+k_2)^{n_2} \cdots (k_1 + \cdots + k_r)^{n_r}}$$

has more than one analytic continuations at non-positive integers. For instance, Sadaoui [29, Thm. 1] used the Raabe's identity while Akiyama and Yanigawa [1, p. 350] considered the Euler-Maclaurin summation formula. Since both results involve Bernoulli number, applying Bernoulli symbol reveals, to our surprise, that both analytic continuations coincide. More precisely, for non-negative integers $n_1, \ldots, n_k$, we have, symbolically,

$$\zeta_r(-n_1, \ldots, -n_r) = \prod_{k=1}^{r} (-1)^{n_k} \mathcal{C}_{1,\ldots,k}^{n_k+1} \tag{3}$$

where $\mathcal{C}_1^n = \mathcal{B}_1^n/n$ and recursively, $\mathcal{C}_{1,\ldots,k+1} = (\mathcal{C}_{1,\ldots,k} + \mathcal{B}_{k+1})^n/n$. This shows the two approaches, by Raabe's identity and Euler-Maclaurin summation formula that lead to analytic continuations of MZVs, coincide on non-positive integer values.

Other results such as recurrence [17, Thm. 3.1], contiguity identities [17, Thm. 4.1], and generating functions [17, Thm. 5.1] follow naturally from (3).

1.3 Orthogonal polynomials

Since $E_n^{(p)}(x)$ can be viewed as the nth moment of certain random variable, it is natural to consider other probabilistic objects, such as the monic orthogonal polynomials, denoted by $\Omega_n^{(p)}(y)$. Here, orthogonality means, for any integers r and n with $0 \le r < n$,

$$y^r \Omega_n^{(p)}(y) \Big|_{y^k = E_k^{(p)}(x)} = 0,$$

where the left-hand sides means expanding the polynomial and evaluating at $y^k = E_k^{(p)}(x)$ for each power of y. In [15], we not only give the recurrence of $\Omega_n^{(p)}(y)$ as

$$\Omega_{n+1}^{(p)}(y) = \left(y - x + \frac{p}{2}\right) \Omega_n^{(p)}(y) + \frac{n(n+p-1)}{4} \Omega_{n-1}^{(p)}(y), \tag{4}$$

but also recognize that $\Omega_n^{(p)}(y) = i^n n! P_n^{\left(\frac{p}{2}\right)}\left(-i\left(y - x + \frac{p}{2}\right); \frac{\pi}{2}\right)/2^n$ for Meixner-Pollaczek polynomial $P_n^{(\lambda)}(y;\phi)$ [23, eq. 9.7.1]. In fact, (4) connects $E_n^{(p)}(x)$ to generalized Motzkin numbers through a continued fraction expression (see [19, Thm. 13]). Namely, define a sequence $\mathfrak{E}_{n,k}^{(p)}$ by $\mathfrak{E}_{0,0}^{(p)} = 1$ and for $n > 0$, by the recurrence

$$\mathfrak{E}_{n+1,k}^{(p)} = \mathfrak{E}_{n,k-1}^{(p)} + \left(x - \frac{p}{2}\right) \mathfrak{E}_{n,k}^{(p)} - \frac{(k+1)(k+p)}{4} \mathfrak{E}_{n,k+1}^{(p)}.$$

Then, when $k = 0$, we have $\mathfrak{E}_{n,0}^{(p)} = E_n^{(p)}(x)$. The weighted lattice paths interpretation [8, p. 319] of generalized Motzkin numbers now can be endowed on $E_n^{(p)}(x)$, giving it a matrix representation [15, Thm. 14]. See also an example [15, Ex. 16], which shows connections between E_n and Catalan number C_n, through weighted lattice paths. Analogue for $B_n(x)$ are also obtained [15, Thm. 17]: let $\varrho_n(y)$ be the monic orthogonal polynomials with respect to $B_n(x)$, i.e., for integers r and n, with $0 \le r < n$, $y^r \varrho_n(y)|_{y^k = B_k(x)} = 0$. Then,

$$\varrho_{n+1}(y) = \left(y - x + \frac{1}{2}\right) \varrho_n(y) + \frac{n^4}{4(2n+1)(2n-1)} \varrho_{n-1}(y). \tag{5}$$

In particular, $\varrho_n(y) = n! p_n\left(y; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)/(n+1)_n$, where $p_n(y; a, b, c, d)$ is the continuous Hahn polynomial [23, pp. 200–202].

1.4 Random walk, Brownian motion, and Bessel process

As a convolution, it is not hard to see that

$$E_n^{(p)}(x) = \sum_{k_1+\cdots+k_p=n} \binom{n}{k_1,\ldots,k_p} E_{k_1}(x)E_{k_2}(0)\cdots E_{k_p}(0).$$

In [19], based on the probabilistic interpretation, we obtained, for any positive integer N,

$$E_n(x) = \frac{1}{N^n}\sum_{l=N}^{\infty} p_l^{(N)} E_n^{(l)}\left(\frac{l-N}{2}+Nx\right),$$

where the coefficients $p_l^{(N)}$ appear in the series expansion of the reciprocal of the Nth Chebychev polynomial of the first kind T_N

$$\frac{1}{T_N(1/z)} = \sum_{\ell=0}^{\infty} p_\ell^{(N)} z^\ell.$$

Moreover, $p_\ell^{(N)}$ can also be viewed as transition probabilities in the context of a random walk over a finite number of sites [19, Note 4.8]. Inspired by this idea, we further explored another probabilistic method in [21]. By considering both 1-dim reflected Brownian motion and 3-dim Bessel process and especially studying the hitting times for consecutive level sites, we obtained several identities involving $B_n^{(p)}(x)$ and $E_n^{(p)}(x)$.

Recently, we [14] extended the loop decomposition from 1 and 2 loop cases into general n loops, by both induction and a combinatorial interpretation. Further identities are derived from equally distributed level sites. For instance, the 3-loop cases in 3-dim Bessel process implies

$$B_{n+1}\left(\frac{x+2}{5}\right) - B_{n+1}\left(\frac{x}{5}\right) = \frac{n+1}{5^n}\sum_{k=0}^{\infty}\frac{3^k}{2^{2k+3}}\sum_{\ell=0}^{k}\binom{k}{\ell}(-1)^\ell\frac{1}{12^\ell}E_n^{(2k+2\ell+3)}(k+\ell+x).$$

1.5 Hankel Determinants and Continued Fractions

Hankel determinants play an essential role in the study of orthogonal polynomials, continued fractions, and the moment problems in probability. Several formulas on Bernoulli and Euler numbers are known; while the one for special subsequences of Bernoulli and Euler Polynomials were open to discover. In a serious of work [5, 6, 7, 13], we obtained the formulas of Hankel determinants of different sequences of numbers and polynomials, all related to Bernoulli and Euler polynomials.

In particular, together with an undergraduate student, we [13] first computed the Hankel determinants of $B_{2n+1}\left(\frac{x+1}{2}\right)/(2n+1)$ and $B_{2n+3}\left(\frac{x+1}{2}\right)/(2n+3)$. On the very next day after posting the result on arXiv, we draw the attention of Prof. Christian Krattenthaler[1] from University of Vienna, an expert in determinants. By seriously taking his valuable suggestions and independently working on his conjecture, we provided alternative proof of the sequence of $B_{2n+5}\left(\frac{x+1}{2}\right)/(2n+5)$. More importantly part of this result can be applied to non-parametric estimations in statistics, especially in [4]. This potential leads to collaboration and applications in statistics.

1.6 Some Future Plans

A long project right now is based on mutual connections among orthogonal polynomials, lattice paths, continued fractions and Hankel determinants; see, e.g., [5, 6, 7, 15]. Shot term aims at

- algorithms in computing operations of continued fraction expressions;
- labeled tree generating polynomials;
- and Hankel determinant guessing and computing.

My further concentration will be the random variable expressions and models in probability; later, the family of Sheffer sequences will be extended beyond only these two polynomials.

- For instance, some recent results, e.g., in [3], Budd studied the square lattice random walk related to Elliptic functions, can be a good start as a new model to explore new identities.
- Those lattice and corresponding tree structures are also related to certain polynomials, especially with labeled trees. This is also an ongoing joint work with Dr. Jun Ma from Shanghai Jiao Tong University.

[1] https://www.mat.univie.ac.at/~kratt/

Meanwhile, I would also involve more computational number theory research. In an early paper [15], we discovered new matrix representations of Bernoulli and Euler polynomials, including some of their extensions to higher-order. Therefore, other matrix representations of classic and new sequences of numbers, polynomials are of important interests.

- My next plan is to combining the probabilistic method, i.e., exploring algorithms with randomized steps; and comparing with quantum computing mechanisms, to modify or discover new, especially quantum, algorithms. The current plan is to begin with algorithms related to integer factorization, sum of squares, and integer partitions, which will be elaborated in the next subsection.
- A second direction is to explore the differential geometry framework in effectively finding quantum gates, for which, see the famous result published in Science [25]. This is my long term direction, also with focus on potential applications in number theory and combinatorics

Another direction involves matrices: matrix representation of certain functions, polynomials, e.g., [15, 16]. Also inspired by recent result [22] of M. Kauers and J. Moosbauer, matrix multiplication still can be improved. I will focus on

- quantum gates that are represented by certain matrices;
- and other calculations of matrices, involving quantum computing.

2 Symbolic and Quantum Computing

In general, computer or machine proofs, as the major aim in symbolic computation, always contribute to mathematical proofs. Bernoulli and Euler symbols mentioned above can also be considered as generalized symbolic computation method.

For the traditional symbolic computation, I mainly concentrate on an integration method, named the Method of Brackets, e.g. [9, 10, 11, 12]. It is an efficient method for the evaluation of a large class of definite integrals on the half-line, i.e.,

$$\int_0^\infty f(x)dx,$$

with only 6 simple rules, and can evaluate complicated integrals. The importance of symbolic integration, as well as symbolic summations, is also due to the applications to evaluate certain Feymann integrals, which arise from Feynman diagrams. In theoretical physics, a Feynman diagram is a pictorial representation of the mathematical expressions describing the behavior and interaction of subatomic particles.

In Summer 2022, I worked with Siyuan Wu, a student of Class of 2023 with the project grant “Implementation on the Method of Brackets”, approved by Duke Kunshan Unversity (DKU) Summer Research Scholars (SRS) program committee. The main project is to implement the algorithm into a package in Mathematica and the continuation leads to comparison among different symbolic integration methods, e.g., negative dimension integration method. This will enlarge the family of tools in evaluating the Feymann integrals, and guide us to find the best method, based on different integrals.

In July 2021, as a Co-PI together with Dr Myung-Joong Hwang, Assistant Professor of Physics at DKU, we are awarded the Interdisciplinary Seed Grant: “Quantum algorithms for computational number theory, linear algebra, and combinatorics”. I focus on quantum algorithms, especially applications in Number Theory. For example, prime factorization for a large integer is always time consuming in practice and Shor’s Algorithm in prime factorization, based on quantum computers, not only dramatically reduces the time needed, also demonstrates that the integer factorization problem can be efficiently solved on a quantum computer.

The ultimate goal is to study and explore the combination of quantum computing, algorithms, and symbolic computations. I am interested in the following important topics, due to their connections among different branches, and the potential applications in many unsolved problems.

- Matrices: such as matrix representations of special functions, numbers. Note that quantum gates are represented by certain matrices, any result for those matrices is crucial to quantum computing. Besides, matrices in general are widely applied in, e.g., data science. My novel approach, by combining quantum computing and special functions brings new aspect in both directions.
- Implementation of Algorithms: including classical and quantum algorithms, so the platform can be Python, Mathematica, and Qiskit. Producing algorithm packages is always important in Experimental Mathematics. For instance, in my previous Research Institute for Symbolic Computations, PhD students are required to implement a package instead of publishing paper(s) in order to graduate. Another reason for this direction is,

undergraduates students in math, computer science, and data science can participate and contribute, under my supervision.

- Differential Geometry: not only because I gained expertise in this during my master's study (see the next section), but also it is a well-know result that to find optimal quantum circuits is essentially equivalent to find the shortest path between two points in a certain curved geometry, i.e., geodesics. This theory [25] interprets quantum gates under the frame of differential geometry. I am working on more practical algorithms, by largely following this algorithm, but with slight modification; in this way, we can improve the algorithm, by still using relative small number of gates, but dramatically reducing the time to find those gates.

3 Differential and Information Geometry.

I studied information geometry for my master's degree. It is the application of differential geometry in probability and statistics. Recently, the theory has been largely applied, in Control Theory, Neural Networks, and Machine Learning. Switching to studying Experimental Mathematics in my PhD program does not prevent me from continuing my research in Information Geometry; See, e.g., [20, 24, 27, 30].

- I contributed to an awarded joint grant "Wuhan University—Duke Kunshan University—University of Minnesota, Twin Cities Joint Research Platform", together with Dr. Dongmian Zou, Assistant Professor of Data Science, DKU.
- As described above the finding optimal quantum circuits under the framework of differential geometry, leads me to re-study this topic, from a different aspect. The current and potential profound applications, the early experience, and collaborations with other colleagues are my key motivations in this area.
- A most recent on-going joint work/draft is on the family of hyperbolic secant distributions $HS\left(\alpha,\rho\right)$, whose probability density function is given by

$$p_{\alpha,\rho}\left(t\right)=C\left(\alpha,\rho\right)\operatorname{sech}^{\rho}\left(\alpha t\right),$$

where, for uniformization,

$$C\left(\alpha,\rho\right)=\frac{1}{\int_{\mathbb{R}}\operatorname{sech}^{\rho}\left(\alpha t\right)dt}=\frac{1}{\frac{2^{\rho-1}}{\alpha}B\left(\frac{\rho}{2},\frac{\rho}{2}\right)}.$$

One essential reason is that the density functions of both Bernoulli and Euler symbols belong to the family. Together with Dr. Linyu Peng, Keio University, we basically use differential and information geometry to study the family of hyperbolic secant densities, which are the densities of Bernoulli and Euler symbols. Once this work is done, we shall continue with how those geometric structures can lead, regarding to the identities, orthogonal polynomials, continued fractions, and any algorithms.

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