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Chapter I Hot Topics in Symbolic Computation

Peter Paule

Lena Kartashova, Manuel Kauers, Carsten Schneider, Franz Winkler

The development of computer technology has brought forth a renaissance of algorithmic mathematics which gave rise to the creation of new disciplines like Computational Mathematics. Symbolic Computation, which constitutes one of its major branches, is the main research focus of the Research Institute for Symbolic Computation (RISC).

In the first Section 1, author P. Paule, one finds an introduction to the theme together with comments on history as well as on the use of the computer for mathematical discovery and proving. The remaining sections of the chapter present more detailed descriptions of hot research topics currently pursued at RISC.

Section 2, author F. Winkler, introduces to algebraic curves; a summary of results in theory and applications (e.g., computer aided design) is given. Section 3, author M. Kauers, reports on computer generated progress in lattice paths theory finding applications in combinatorics and physics. Section 4, author C. Schneider, provides a description of an interdisciplinary research project with DESY (Deutsches Elektronen-Synchrotron, Berlin/Zeuthen). Section 5, author E. Kartashova, describes the development of Nonlinear Resonance Analysis, a new branch of mathematical physics.

The Renaissance of Algorithmic Mathematics 1

"The mathematics of Egypt, of Babylon, and of the ancient Orient was all of the algorithmic type. Dialectical mathematics-strictly logical, deductive mathematics-originated with the Greeks. But it did not displace the algorithmic. In Euclid, the role of dialectic is to justify a construction-i.e., an algorithm. It is only in modern times that we find mathematics with little

or no algorithmic content. [...] Recent years seem to show a shift back to a constructive or algorithmic view point."

To support their impression the authors of [DH81] continue by citing P. Henrici: "We never could have put a man on the moon if we had insisted that the trajectories should be computed with dialectic rigor. [...] Dialectic mathematics generates insight. Algorithmic mathematics generates results."

Below we comment on various aspects of recent developments, including topics like numerical analysis versus symbolic computation, and pure versus applied mathematics. Then we present mathematical snapshots which-from symbolic computation point of view-shed light on two fundamental mathematical activities, discovery (computer-assisted guessing) and proving (using computing algebra algorithms).

1.1 A Bit of History

We will high-light only some facets of the *recent* history of algorithmic mathematics. However, we first need to clarify what algorithmic mathematics is about.

Algorithmic vs. Dialectic Mathematics

About thirty years ago P.J. Davis and R. Hersh in their marvelous book [DH81] included a short subsection with exactly the same title. We only make use of their example (finding $\sqrt{2}$) to distinguish between algorithmic and dialectic (i.e. non-algorithmic) mathematics. But to the interested reader we recommend the related entries of [DH81] for further reading.

Consider the problem to find a solution, denoted by $\sqrt{2}$, to the equation $x^2 = 2$.

Solution 1

Consider the sequence $(x_n)_{n\geq 1}$ defined for $n\geq 1$ recursively by

$$x_{n+1} = \frac{1}{2} \left(x_n + \frac{2}{x_n} \right),$$

with initial value $x_1 = 1$. Then $(x_n)_{n \geq 0}$ converges to $\sqrt{2}$ with quadratic rapidity. For example, $x_4 = \frac{577}{408} = 1.414215\ldots$ is already correct to 5 decimal places. Note, the algorithm can be carried out with just addition and division, and without complete theory of the real number system.

Solution 2

Consider the function $f(x) = x^2 - 2$ defined on the interval from 0 to 2. Observe that f is a continuous function with f(0) = -2 and f(2) = 2. Therefore, according to the intermediate value theorem, there exists a real number, let's call it $\sqrt{2}$, such that $f(\sqrt{2}) = 0$. Note, the details of the argument are based on properties of the real number system.

Solution 1 is algorithmic mathematics; solution 2 is the dialectic solution. Note that, in a certain sense, neither solution 1 nor solution 2 is a solution at all. Solution 1 gives us a better and better approximation, but no x_n gives us an exact solution. Solution 2 tells us that an exact solution exists between 0 and 2, but that is all it has to say.

Numerical Analysis vs. Symbolic Computation

Readers interested in the relatively young history of symbolic computation are refered to respective entries in the books [GCL92] and [vzGG99]. Concerning the first research journal in this field, [vzGG99] says, "The highly successful Journal of Symbolic Computation, created in 1985 by Bruno Buchberger, is the undisputed leader for research publication." So in 1981 when the book [DH81] appeared, symbolic computation was still at a very early stage of its development. This is reflected by statements like: "Certainly the algorithmic approach is called for when the problem at hand requires a numerical answer which is of importance for subsequent work either inside or outside mathematics."

Meanwhile this situation has changed quite a bit. Nowadays, symbolic computation and numerical analysis can be viewed as two sides of the same medal, i.e. of algorithmic mathematics. In other words, until today also symbolic computation has developed into a discipline which provides an extremely rich tool-box for problem solving outside or inside mathematics. Concerning the latter aspect, in view of recent applications, including some being described in the sections of this chapter, symbolic computation seems to evolve into a key technology in mathematics.

In fact there are numerous 'problems at hand' which for subsequent (e.g. numerical) work greatly benefit from simplification produced by symbolic computation algorithms. As a simple example, let us consider the problem of adding the first n natural numbers, i.e., to compute the sum

$$x_n := 1 + 2 + \dots + n = \sum_{k=1}^{n} k.$$

Solution A

Consider the sequence $(x_n)_{n\geq 1}$ defined for $n\geq 1$ recursively by

$$x_{n+1} = x_n + n + 1,$$

with initial value $x_1 = 1$. In other words, this computes the sum x_n by carrying out n - 1 additions. For example, $x_4 = x_3 + 4 = (x_2 + 3) + 4 = ((x_1 + 2) + 3) + 4 = 10$.

Solution B

Apply a symbolic summation algorithm (e.g., Gosper's algorithm implemented in most of the computer algebra systems) to *simplify* the sum; i.e., which finds that for $n \ge 1$,

$$x_n = \frac{1}{2}n(n+1).$$

Instead of carrying out n-1 additions, this computes the sum x_n by one multiplication and one division by 2. For example, $x_4 = \frac{1}{2}4 \cdot 5 = 10$. In other words, a symbolic computation reduces the numerical task from n-1 operations (additions) to 2!

There are many problems for which better solutions would be obtained by a proper *combination* of numerical analysis with symbolic computation. Such kind of research was the main theme of the Special Research Program SFB F013 Numerical and Symbolic Scientific Computing (1998-2008), an excellence program of the Austrian Science Funds FWF, pursued by groups at RISC, from numerical analysis and applied geometry at the Johannes Kepler University (JKU), and at the Johann Radon Institute of Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences. Starting in October 2008 this initiative has been continued at the JKU in the form of the Doctoral Program Computational Mathematics, another excellence program of the FWF.

Pure vs. Applied Mathematics

Efforts in numerical analysis and symbolic computation to combine mathematics with the powers of the computer are continuing to revolutionize mathematical research. For instance, as mentioned above, a relatively young mathematical field like symbolic computation is growing more and more into the role of a key technology within mathematics. As a by-product the distinction between 'pure' and 'applied' mathematics is taking on a less and less

definite form. This stays quite in contrast to a period in the younger history of mathematics.



G. H. Hardy (1877-1947). From http://en.wikipedia.org/wiki/File:Ghhardy@72.jpg

Figure 1

The famous mathematician G.H. Hardy (1877-1947) insisted that all of the mathematics he created during his life time was of no use at all. In the concluding pages of his remarkable Apology [Har40] he wrote, "I have never done anything 'useful'. No discovery of mine has made, or is likely to make, directly or indirectly, for good or for ill, the least difference to the amenity of the world. I have helped to train other mathematicians, but mathematicians of the same kind as myself, and their work has been, so far at any rate as I have helped them to it, as useless as my own. Judged by all practical standards, the value of my mathematical life is nil." During that time a pervasive unspoken sentiment began to spread, namely that there is something ugly about applications. To see one of the strongest statements about purity, let us again cite G.H. Hardy [Har40], "It is undeniable that a good deal of elementary mathematics [...] has considerable practical utility. These parts of mathematics are, on the whole, rather dull; they are just the parts which have least aesthetic value. The 'real' mathematics of the 'real' mathematicians, the mathematics of Fermat and Euler and Gauss and Abel and Riemann, is almost wholly 'useless'."

This attitude, often called Hardyism, was "central to the dominant ethos of twentieth-century mathematics" [DH81]. Only towards the end of the sev-

enties this credo began to soften up due to the beginning evolution of computer technology. Bruno Buchberger has been one of the pioneers in this development. Since he became JKU Professor in 1974 he has been pushing and promoting the central role of computer mathematics. With the rapid dissemination of computer technology such ideas were taken up. Attractive positions were created, and the reputation of 'applied' mathematics was increasing. Starting with this process in the U.S.A., the full wave of this development came back to Europe with some delay. Let me cite from a recent article [Due08] of Gunter Dueck, who in 1987 moved to IBM from his position of a mathematics professor at the university of Bielefeld: "Rainer Janssen (mein damaliger Manager bei IBM und heute CIO der Muenchner Rueck) und ich schrieben im Jahre 1991 einen Artikel mit dem Titel 'Mathematik: Esoterik oder Schluesseltechnologie?' Dort stand ich noch echt unter meinem Zorn, als Angewandter Mathematiker ein triviales Nichts zu sein, welches inexakte Methoden in der Industrie ganz ohne Beweis benutzt und mit Millioneneinsparungen protzt, obwohl gar nicht bewiesen werden kann, dass die gewaehlte Methode die allerbeste gewesen ist."

Nowadays the situation is about to change fundamentally. Things have been already moved quite a bit. For example, today 'hardyists' would say that working in algorithmic mathematics is almost impossible without running into concrete applications! Conrete examples can be found in the sections below, in particular, in Section 4 which describes the use of symbolic summation in particle physics.

To be fair to Hardy one should mention that despite his 'hardyistic' statements, he was following with interest modern developments, for example, that of computing machines. In particular, he was appreciating the work of Alan Turing. Thanks to Hardy's recommendation, the Royal Society awarded Turing 40 English pounds for the construction of a machine to compute the zeros of the Riemann zeta function [dS04].

Before coming to the mathematical part of this section, another quote of G. Dueck [Due08]: "Damals forderten Rainer Janssen und ich, dass Mathematik sich als Schluesseltechnologie begreifen sollte. [...] Ja, Mathematik ist eine Schluesseltechnologie, aber eine unter recht vielen, die alle zusammen multi-kulturell ein Ganzes erschaffen koennen. Die Mathematik muss sich mit freudigem Herzen diesem Ganzen widmen - dem Leben. Sie muss sich nach aussen verpflichtet zeigen, den Menschen und dem Leben etwas Wichtiges zu sein und zu bringen." It is exactly this attitude that one can find at a place like the Softwarepark Hagenberg.

7

Computer-Assisted Discovery and Proving 1.2

First we comment on *computer-assisted guessing* in the context of mathematical discovery. Then we turn to the activity of proving, more precisely, to *proving methods* where *computer algebra algorithms* are used. Here we restrict to this special type of computed-assisted proving; for *general mathematical proving machines* like the THEOREMA system developed at RISC, see Chapter ??.

I.Q. Tests, Rabbits, and the Golden Section

Let us consider the following problem taken from an I.Q. test [Eys66, Aufgabe 13, Denksport I fuer Superintelligente] from the sixties of the last century:

```
Continue the sequence 1, 1, 2, 3, 5, 8, 13, 21.
```

In the 21st century we let the computer do the problem. To this end we load the RISC package GeneratingFunctions written by C. Mallinger [Mal96a] in the computer algebra system Mathematica:

```
\operatorname{In}[1] := \ll \operatorname{GeneratingFunctions.m}
```

In the next step we input a little program that can be used to solve such I.Q. tests automatically:

```
\begin{split} & \ln[2] \!\! := \mathtt{GuessNext2Values[Li\_]} \; := \; \mathtt{Module[\{rec\},} \\ & \quad \mathsf{rec} \; = \; \mathtt{GuessRE[Li,c[k],\{1,2\},\{0,3\}]}; \\ & \quad \mathsf{RE2L[rec[[1]],c[k],Length[Li]+1]]} \end{split}
```

Finally the problem is solved automatically with

```
\begin{split} & \text{In}[3] \! := \texttt{GuessNext2Values}[\{1,1,2,3,5,8,13,21\}] \\ & \text{Out}[3] \! = \{1,1,2,3,5,8,13,21,34,55\} \end{split}
```

To produce additional values is no problem:

```
\begin{split} & \text{In}[4] \!:= \texttt{GuessNext2Values}[\{1,1,2,3,5,8,13,21,34,55\}] \\ & \text{Out}[4] \!= \{1,\!1,\!2,\!3,\!5,\!8,\!13,\!21,\!34,\!55,\!89,\!144\} \end{split}
```

Note. The same automatic guessing can be done in the Maple system; there B. Salvy and P. Zimmermann [SZ94] developed the poineering package gfun which has served as a model for the development of Mallinger's GeneratingFunctions.

What is the mathematical basis for such automatic guessing? The answer originates in a simple observation: Many of the sequences $(x_n)_{n\geq 0}$ arising in

practical applications (and in I.Q. tests!) are produced from a very simple pattern; namely, linear recurrences of the form

$$p_d(n)x_{n+d} + p_{d-1}(n)x_{n+d-1} + \dots + p_0(n)x_n = 0, \qquad n \ge 0,$$

with coefficients $p_i(n)$ being polynomials in n. So packages like Mallinger's GeneratingFunctions try to compute-via an ansatz using undetermined coefficients-a recurrence of exactly this type. For the I.Q. example above a recurrence is obtained by

$$\begin{split} & \text{In}[5] := \texttt{GuessRE}[\{1,1,2,3,5,8,13,21\},\texttt{f}[\texttt{k}]] \\ & \text{Out}[5] = \{\{-f[\texttt{k}]-f[1+\texttt{k}]+f[2+\texttt{k}]==0,f[0]==1,f[1]==1\},\text{ogf}\} \end{split}$$

Since only finitely many values are given as input, the output recurrence $f_{n+2} = f_{n+1} + f_n$ $(n \ge 0)$ can be only a guess about a possible building principle of an infinite sequence. However, such kind of automated guessing is becoming more and more relevant to concrete applications. For instance, an application from mathematical chemistry can be found in [CGP99] where a prediction for the total number of benzenoid hydrocarbons was made. Three years later this predication was confirmed [VGJ02]. Recently, quite sophisticated applications arose in connection with the enumeration of lattice paths, see Section 3, and also with quantum field theory, see Section 4.

In 1202 Leonard Fibonacci introduced the numbers f_n . The fact that $f_0 = f_1 = 1$, and

$$f_{n+2} = f_{n+1} + f_n, \qquad n \ge 0,$$

in Fibonacci's book was given the following interpretation: If baby rabbits become adults after one month, and if each pair of adult rabbits produces one pair of baby rabbits every month, how many pairs of rabbits, starting with one pair, are present after n months?

A non-recursive representation is the celebrated Euler-Binet formula

$$f_n = \frac{1}{\sqrt{5}} \left(\left(\frac{1+\sqrt{5}}{2} \right)^{n+1} - \left(\frac{1-\sqrt{5}}{2} \right)^{n+1} \right), \quad n \ge 0.$$

The number $(1+\sqrt{5})/2 \approx 1.611803$, the golden ratio, is important in many parts of mathematics as well as in the art world. For instance, Phidias is said to have used it consciously in his sculpture.

Mathematicians gradually began to discover more and more interesting things about Fibonacci numbers f_n ; see e.g. [GKP94]. For example, a typical sunflower has a large head that contains spirals of tightly packed florets, usually with $f_8 = 34$ winding in one direction and $f_9 = 55$ in another.

Another observation is this: Define g_n as a sum over binomial coefficients of the form

$$g_n := \sum_{k=0}^n \binom{n-k}{k}.$$

From the values $g_0 = 1$, $g_1 = 1$, $g_2 = 2$, $g_3 = 3$, $g_4 = 5$, and $g_5 = 8$ it is straight-forward to conjecture that the sequence $(g_n)_{n\geq 0}$ is nothing but the Fibonacci sequence $(f_n)_{n\geq 0}$. In the next subsection we shall see that nowadays such statements can be proved automatically with the computer.

Pi, Inequalities, and Finite Elements

We have seen that linear recurrences can be used as a basis for automated guessing. Concerning symbolic computation, this is only the beginning. Namely, following D. Zeilberger's holonomic paradigm [Zei90b], the description of mathematical sequences in terms of linear recurrences, and of mathematical functions in terms of linear differential equations, is also of great importance to the design of computer algebra algorithms for automated proving.

For example, consider the sequence $(g_n)_{n\geq 0}$ defined above. To prove the statement

$$f_n = g_n, \qquad n \ge 0,$$

in completely automatic fashion, we use the RISC package Zb[PS95a], an implementation of D. Zeilberger's algorithm [Zei90a]:

$$In[6] := \ll Zb.m$$

$$\begin{split} & \text{In}[7] \!:= \text{Zb}\left[\text{Binomial}\left[\text{n-k,k}\right], \left\{\text{k,0,Infinity}\right\}, \text{n,2}\right] \\ & \text{Out}[7] \!= \left\{\text{SUM}[n] + \text{SUM}[1+n] - \text{SUM}[2+n] == 0\right\} \end{split}$$

The output tells us that $g_n = \text{SUM}[n]$ indeed satisfies the same recurrence as the Fibonacci numbers. A proof for the correctness of the output recurrence can be obtained automatically, too; just type the command:

$$In[8]:= Prove[]$$

For further details concerning the mathematical background of this kind of proofs, see e.g. Zeilberger's articles [Zei90b] and [Zei90a] which were the booster charge for the development of a new subfield of symbolic computation; namely, the design of computer algebra algorithms for special functions and sequences. For respective RISC developments the interested reader is referred to the web page

For various applications researchers are using such algorithms in their daily research work-sometimes still in combination with tables. However, there are

particular problem classes where symbolic (and numeric) algorithms are going to replace tables almost completely.

Concerning special sequences the most relevant table is N. Sloane's handbook [Slo73], [Slo94]. Sloane's home page provides an extended electronic version of it; also symbolic computation algorithms are used to retrieve information about sequences .

Concerning special functions one of the most prominent tables is the 'Handbook' [AS64] from 1964. Soon it will be replaced by its strongly revised successor, the NIST Digital Library of Mathematical Functions; see http://dlfm.nist.gov. The author of this section is serving as an associate editor of this new handbook (and author, together with F. Chyzak, of a new chapter on computer algebra) that will be freely available via the web.

We expect the development of special provers will intensify quite a bit. By special provers we mean methods based on computer algebra algorithms specially tailored for certain families of mathematical objects. *Special function inequalities* provide a classical domain that so far has been considered as being hardly accessible by such methods. To conclude this section we briefly describe that currently this situation is about to change.

Consider the famous Wallis product formula for π :

$$\pi = 2 \cdot \frac{2}{1} \cdot \frac{2}{3} \cdot \frac{4}{3} \cdot \frac{4}{5} \cdot \frac{6}{5} \cdot \frac{6}{7} \cdot \frac{8}{7} \cdot \frac{8}{9} \cdot \cdots$$

This product is an immediate consequence $(n \to \infty)$ of the following inequality (JohnWallis, Arithmetica Infinitorum, 1656):

$$\frac{2n}{2n+1} \le \frac{c_n}{\pi} \le 1, \qquad n \ge 0,$$

where

$$c_n := \frac{2^{4n+1}}{2n+1} \binom{2n}{n}^{-2}.$$

In analysis one meets such inequalities quite frequently. Another example, similar to that of Wallis, is

$$\frac{1}{4n} \le a_n \le \frac{1}{3n+1}, \qquad n \ge 0,$$

where

$$a_n := \frac{1}{2^{4n}} \binom{2n}{n}^2.$$

We shall prove the right hand side, i.e. $a_n \leq 1/(3n+1)$, (the left hand side goes analogously) to exemplify the new Gerhold-Kauers method [GK05] for proving special function/sequence inequalities. As proof strategy they use mathematical induction combined with G. Collins' cylindrical algebraic decomposition (CAD). First observe that

$$a_{n+1} = a_n \frac{(2n+1)^2}{(2n+2)^2} \le \frac{1}{3n+1} \frac{(2n+1)^2}{(2n+2)^2},$$

where for the inequality the induction hypothesis is used. In order to show that this implies $a_{n+1} \leq 1/(3n+4)$, it is sufficient to establish that

$$\frac{1}{3n+1} \frac{(2n+1)^2}{(2n+2)^2} \le \frac{1}{3n+4}.$$

But this step can be carried out automatically with any implementation of Collins' CAD; for instance, in Mathematica:

$$\begin{split} & \text{In}[9] \! := \mathtt{Reduce} \, [\, \frac{1}{3n+1} \, \frac{(2n+1)^2}{(2n+2)^2} \leq \frac{1}{3n+4}, n] \\ & \text{Out}[9] \! = -\frac{4}{3} < n < -1 \mid \mid -1 < n < -\frac{1}{3} \mid \mid n \geq 0 \end{split}$$

The Gerhold-Kauers method already found quite a number of non-trivial applications. They range from new refinements of Wallis' inequality [PP08] like

$$\frac{32n^2 + 32n + 7}{4(2n+1)(4n+3)} \le \frac{c_n}{\pi} \le \frac{16(n+1)(2n+1)}{32n^2 + 56n + 25}, \qquad n \ge 0,$$

to a proof of the long-standing log-concavity conjecture of V. Moll [KP07]. Further applications and details about the method are given in [Kau08].

We want to conclude by referring to results that emerged from numerical-symbolic SFB collaboration in the context of finite element methods (FEM). In order to set up a new FEM setting, J. Schoeberl (RWTH Aachen, formerly JKU) needed to prove the following special function inequality:

$$\sum_{j=0}^{n} (4j+1)(2n-2j+1)P_{2j}(0)P_{2j}(x) \ge 0$$

for $-1 \le x \le 1$, $n \ge 0$, and with $P_{2j}(x)$ being the Legendre polynomials. Using the Gerhold-Kauers method together with RISC symbolic summation software, V. Pillwein [Pil07] was able to settle this conjecture. Remarkably, there is still no human proof available!

Last but not least, we mention a recent collaboration of J. Schoeberl with C. Koutschan (RISC), which led to a new tool for engineering applications in the context of electromagnetic wave simulation. Formulas derived by Koutschan's symbolic package HolonomicFunctions resulted in a significant speed-up of numerical FEM algorithms e.g. for the construction of antennas or mobile phones. The method is planned to be registered as a patent.

2 Rational Algebraic Curves – Theory and Application

What is a Rational Algebraic Curve?

A plane algebraic curve C is the zero locus of a bivariate square-free polynomial f(x, y) defined over a field K; i.e.

$$C = \{(a,b) | f(a,b) = 0 \}.$$

More specifically, we call such a curve an affine curve, and the ambient plane the affine plane over K, denoted by $\mathbb{A}^2(K)$. By adding points at infinity for every direction in the affine plane, we get the projective plane over K, denoted by $\mathbb{P}^2(K)$. Points in $\mathbb{P}^2(K)$ have (non-unique) projective coordinates (a:b:c) with $(a,b,c) \neq (0,0,0)$. In projective space only the ratio of the coordinates is fixed; i.e. if $\lambda \neq 0$ then (a:b:c) and $(\lambda a:\lambda b:\lambda c)$ denote the same point in $\mathbb{P}^2(K)$. A projective plane curve $\hat{\mathcal{C}}$ is the zero locus of a homogeneous bivariate square-free polynomial F(x,y,z) over K; i.e.

$$\hat{C} = \{ (a:b:c) | F(a,b,c) = 0 \}.$$

An algebraic curve in higher dimensional affine or projective space is the image of a birational map from the plane into this higher dimensional space. In this paper we concentrate on plane algebraic curves. Algebraic curves in higher dimensional space can be treated by considering a suitable birational image in the plane.

For more detailled information on the topics treated in this paper we refer to [SWa08]. Most of the material for this survey has been developed by the author together with J.Rafael Sendra.

Some plane algebraic curves can be expressed by means of rational parametrizations, i.e. pairs of univariate rational functions. For instance, the tacnode curve (cf. Figure 2) defined in $\mathbb{A}^2(\mathbb{C})$ by the polynomial equation

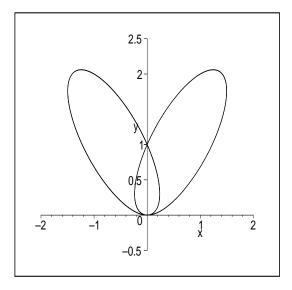
$$f(x,y) = 2x^4 - 3x^2y + y^2 - 2y^3 + y^4 = 0$$

can be represented as

$$\left\{ \left(\frac{t^3 - 6t^2 + 9t - 2}{2t^4 - 16t^3 + 40t^2 - 32t + 9}, \quad \frac{t^2 - 4t + 4}{2t^4 - 16t^3 + 40t^2 - 32t + 9} \right) \; \middle| \; t \in \mathbb{C} \right\}.$$

However, not all plane algebraic curves can be rationally parametrized, for instance the elliptic curve defined by $f(x,y) = x^3 + y^3 - 1$ in $\mathbb{A}^2(\mathbb{C})$.

Definition 1. The affine curve C in $\mathbb{A}^2(K)$ defined by the square–free polynomial f(x,y) is rational (or parametrizable) if there are rational functions



The Tacnode curve

FIGURE 2

 $\chi_1(t), \chi_2(t) \in K(t)$ such that for almost all $t_0 \in K$ (i.e. for all but a finite number of exceptions) the point $(\chi_1(t_0), \chi_2(t_0))$ is on \mathcal{C} , and for almost every point $(x_0, y_0) \in \mathcal{C}$ there is a $t_0 \in K$ such that $(x_0, y_0) = (\chi_1(t_0), \chi_2(t_0))$. In this case $(\chi_1(t), \chi_2(t))$ is called an affine rational parametrization of \mathcal{C} .

Analogously we define projective rational curves.

Some Basic Facts

Fact 1. The notion of rational parametrization can be stated by means of rational maps. More precisely, let C be a rational affine curve and $P(t) \in K(t)^2$ a rational parametrization of C. The parametrization P(t) induces the rational map

$$\mathcal{P}: \mathbb{A}^1(K) \longrightarrow \mathcal{C}$$
$$t \longmapsto \mathcal{P}(t),$$

and $\mathcal{P}(\mathbb{A}^1(K))$ is a dense (in the Zariski topology) subset of \mathcal{C} . Sometimes, by abuse of notation, we also call this rational map a rational parametrization of \mathcal{C} .

Fact 2. Every rational parametrization $\mathcal{P}(t)$ defines a monomorphism from the field of rational functions $K(\mathcal{C})$ to K(t) as follows:

$$\varphi: K(\mathcal{C}) \longrightarrow K(t)$$

 $R(x,y) \longmapsto R(\mathcal{P}(t)).$

Fact 3. Every rational curve is irreducible; i.e. defined by an irreducible polynomial.

Fact 4. Let C be an irreducible affine curve and C^* its corresponding projective curve. Then C is rational if and only if C^* is rational. Furthermore, a parametrization of C can be computed from a parametrization of C^* and vice versa.

Fact 5. Let C be an affine rational curve over K, f(x,y) its the defining polynomial, and $\mathcal{P}(t) = (\chi_1(t), \chi_2(t))$ a rational parametrization of C. Then, there exists $r \in \mathbb{N}$ such that $\operatorname{res}_t(H_1^{\mathcal{P}}(t,x), H_2^{\mathcal{P}}(t,y)) = (f(x,y))^r$.

Fact 6. An irreducible curve C, defined by f(x,y), is rational if and only if there exist rational functions $\chi_1(t), \chi_2(t) \in K(t)$, not both constant, such that $f(\chi_1(t), \chi_2(t)) = 0$. In this case, $(\chi_1(t), \chi_2(t))$ is a rational parametrization of C.

Fact 7. An irreducible affine curve C is rational if and only if the field of rational functions on C, i.e. K(C), is isomorphic to K(t) (t a transcendental element).

Fact 8. An affine algebraic curve C is rational if and only if it is birationally equivalent to K (i.e. the affine line $\mathbb{A}^1(K)$).

Fact 9. If an algebraic curve C is rational then genus(C) = 0.

Proper Parametrizations

Definition 2. An affine parametrization $\mathcal{P}(t)$ of a rational curve \mathcal{C} is *proper* if the map

$$\mathcal{P}: \mathbb{A}^1(K) \longrightarrow \mathcal{C}$$
$$t \longmapsto \mathcal{P}(t)$$

is birational, or equivalently, if almost every point on \mathcal{C} is generated by exactly one value of the parameter t. We define the *inversion* of a proper parametrization $\mathcal{P}(t)$ as the inverse rational mapping of \mathcal{P} , and we denote it by \mathcal{P}^{-1} .

Analogously we define proper projective parametrizations.

Based on Lüroth's Theorem we can see that every rational curve which can be parametrized at all, can be properly parametrized.

Fact 10. Every rational curve can be properly parametrized.

Proper parametrizations can be characterized in many ways; we list some of the more practically usefull characterizations.

Fact 11. Let C be an affine rational curve defined over K with defining polynomial $f(x,y) \in K[x,y]$, and let $P(t) = (\chi_1(t), \chi_2(t))$ be a parametrization of C. Then, the following statements are equivalent:

- 1. $\mathcal{P}(t)$ is proper.
- 2. The monomorphism $\varphi_{\mathcal{P}}$ induced by \mathcal{P} is an isomorphism.

$$\varphi_{\mathcal{P}}: K(\mathcal{C}) \longrightarrow K(t)$$

 $R(x,y) \longmapsto R(\mathcal{P}(t)).$

3.
$$K(\mathcal{P}(t)) = K(t)$$
.
4. $\deg(\mathcal{P}(t)) = \max\{\deg_x(f), \deg_y(f)\}$.

Furthermore, if $\mathcal{P}(t)$ is proper and $\chi_1(t)$ is non-zero, then $\deg(\chi_1(t)) = \deg_y(f)$; similarly, if $\chi_2(t)$ is non-zero then $\deg(\chi_2(t)) = \deg_x(f)$.

Example 3. We consider the rational quintic curve C defined by the polynomial $f(x,y) = y^5 + x^2y^3 - 3x^2y^2 + 3x^2y - x^2$. By the previous theorem, any proper rational parametrization of C must have a first component of degree 5, and a second component of degree 2. It is easy to check that

$$\mathcal{P}(t) = \left(\frac{t^5}{t^2 + 1}, \frac{t^2}{t^2 + 1}\right)$$

properly parametrizes C. Note that $f(\mathcal{P}(t)) = 0$.

A Parametrization Algorithm

We start with the easy case of curves having a singular point of highest possible multiplicity; i.e. irreducible curves of degree d having a point of multiplicity d-1.

Theorem 4 (curves with point of high multiplicity). Let C be an irreducible projective curve of degree d defined by the polynomial $F(x,y,z) = f_d(x,y) + f_{d-1}(x,y)z$ (f_i a form of degree i, resp.), i.e. having a (d-1)-fold point at (0:0:1). Then C is rational and a rational parametrization is $\mathcal{P}(t) = (-f_{d-1}(1,t), -tf_{d-1}(1,t), f_d(1,t))$.

Corollary 5. Every irreducible curve of degree d with a (d-1)-fold point is rational; in particular, every irreducible conic is rational.

Example 6.

- 1. Let \mathcal{C} be the affine ellipse defined by $f(x,y) = x^2 + 2x + 2y^2 = 0$. So, a parametrization of \mathcal{C} is $\mathcal{P}(t) = (-1 + 2t^2, -2t, 1 + 2t^2)$.
- 2. Let \mathcal{C} be the affine quartic curve defined by (see Figure 3)

$$f(x,y) = 1 + x - 15x^2 - 29y^2 + 30y^3 - 25xy^2 + x^3y + 35xy + x^4 - 6y^4 + 6x^2y = 0.$$

 \mathcal{C} has an affine triple point at (1,1). By moving this point to the origin,

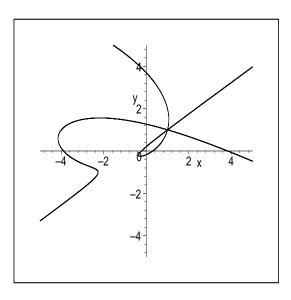


Figure 3 Quartic C

applying the theorem, and inverting the transformation, we get the rational parametrization of ${\mathcal C}$

$$\mathcal{P}(t) = \left(\frac{4+6\,t^3-25\,t^2+8\,t+6\,t^4}{-1+6\,t^4-t}, \frac{4\,t+12\,t^4-25\,t^3+9\,t^2-1}{-1+6\,t^4-t}\right).$$

So curves with a point of highest possible multiplicity can be easily parametrized. But now let $\mathcal C$ will be an arbitrary irreducible projective curve of degree d>2 and genus 0.

Definition 7. A linear system of curves \mathcal{H} parametrizes \mathcal{C} iff

- 1. $\dim(\mathcal{H}) = 1$,
- 2. the intersection of a generic element in \mathcal{H} and \mathcal{C} contains a non-constant point whose coordinates depend rationally on the free parameter in \mathcal{H} ,
- 3. C is not a component of any curve in H.

In this case we say that C is parametrizable by H.

Theorem 8. Let F(x, y, z) be the defining polynomial of C, and let H(t, x, y, z) be the defining polynomial of a linear system $\mathcal{H}(t)$ parametrizing C. Then, the proper parametrization $\mathcal{P}(t)$ generated by $\mathcal{H}(t)$ is the solution in $\mathbb{P}^2(K(t))$ of the system of algebraic equations

$$pp_t(res_y(F, H)) = 0 pp_t(res_x(F, H)) = 0$$

Theorem 9. Let C be a projective curve of degree d and genus 0, let $k \in \{d-1, d-2\}$, and let S_k be a set of kd - (d-1)(d-2) - 1 simple points on C. Then

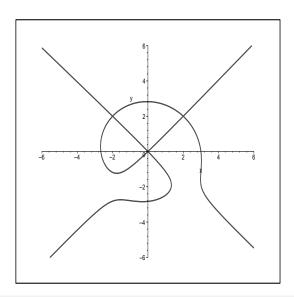
$$\mathcal{A}_k(\mathcal{C}) \cap \mathcal{H}(k, \sum_{P \in \mathcal{S}_k} P)$$

(i.e. the system of adjoint curves of degree k passing through S_k) parametrizes C.

Example 10. Let $\mathcal C$ be the quartic over $\mathbb C$ (see Figure 4) of equation

$$F(x,y,z) = -2xy^2z - 48x^2z^2 + 4xyz^2 - 2x^3z + x^3y - 6y^4 + 48y^2z^2 + 6x^4.$$

The singular locus of C is



$$\operatorname{Sing}(\mathcal{C}) = \{(0:0:1), (2:2:1), (-2:2:1)\},\$$

all three points being double points. Therefore, genus(\mathcal{C}) = 0, and hence \mathcal{C} is rational.

We proceed to parametrize the curve. The defining polynomial of $\mathcal{A}_2(\mathcal{C})$ (adjoint curves of degree 2) is

$$H(x, y, z) = (-2a_{02} - 2a_{20})yz + a_{02}y^2 - 2a_{11}xz + a_{1,1}xy + a_{20}x^2.$$

We choose a set $S \subset (C \setminus \operatorname{Sing}(C))$ with 1 point, namely $S = \{(3:0:1)\}$. We compute the defining polynomial of $\mathcal{H} := A_2(C) \cap \mathcal{H}(2,Q)$, where Q = (3:0:1). This leads to

$$H(x, y, z) = (-2a_{02} - 2a_{20})yz + a_{02}y^2 - 3a_{20}xz + \frac{3}{2}a_{20}xy + a_{20}x^2.$$

Setting $a_{02} = 1$, $a_{20} = t$, we get the defining polynomial

$$H(t, x, y, z) = (-2 - 2t)yz + y^{2} - 3txz + \frac{3}{2}txy + tx^{2}$$

of the parametrizing system. Finally, the solution of the system defined by the resultants provides the following affine parametrization of C

$$\mathcal{P}(t) = \left(12 \frac{9 t^4 + t^3 - 51 t^2 + t + 8}{126 t^4 - 297 t^3 + 72 t^2 + 8 t - 36}, -2 \frac{t(162 t^3 - 459 t^2 + 145 t + 136)}{126 t^4 - 297 t^3 + 72 t^2 + 8 t - 36}\right).$$

Applications of Curve Parametrization

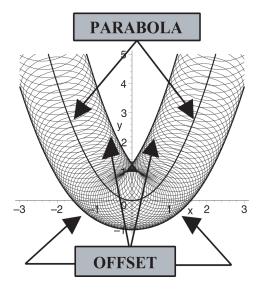
Curve parametrizations can be used to solve certain types of Diophantine equations. For further details on this application we refer to [PV00], [PV02].

Curve paramatrizations can also be used to determine general solutions of first order ordinary differential equations. This is described in [FG04], [FG06].

Many problems in computer aided geometric design (CAGD) can be solved by parametrization. The widely used Bézier curves and surfaces are typical examples of rational curves and surfaces. Offsetting and blending of such geometrical objects lead to interesting problems.

The notion of an offset is directly related to the concept of an envelope. More precisely, the offset curve, at distance d, to an irreducible plane curve $\mathcal C$ is "essentially" the envelope of the system of circles centered at the points of $\mathcal C$ with fixed radius d (see Figure 5). Offsets arise in practical applications such as tolerance analysis, geometric control, robot path-planning and numerical-control machining problems.

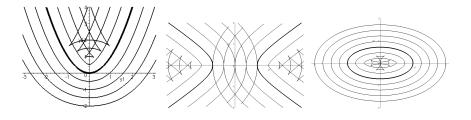
In general the rationality of the original curve is not preserved in the transition to the offset. For instance, while the parabola, the ellipse, and the



Generation of the offsets to the parabola

FIGURE 5

hyperbola are rational curves (compare Figure 6), the offset of a parabola is rational but the offset of an ellipse or a hyperbola is not rational.



Offsets to the parabola (left), to the hyperbola (center), to the ellipse (right)

Figure 6

Let $\mathcal C$ be the original rational curve and let

$$\mathcal{P}(t) = (P_1(t), P_2(t))$$

be a proper rational parametrization of C.

We determine the normal vector associated to the parametrization $\mathcal{P}(t)$, namely

$$\mathcal{N}(t) := (-P_2^{'}(t), P_1^{'}(t)).$$

Note that the offset at distance d basically consist of the points of the form

$$\mathcal{P}(t) \pm \frac{d}{\sqrt{P_1'(t)^2 + P_2'(t)^2}} \mathcal{N}(t).$$

Now we check whether this parametrization satisfies the "rational Pythagorean hodograph condition", i.e. whether

$$P_{1}^{'}(t)^{2} + P_{2}^{'}(t)^{2},$$

written in reduced form, is the square of a rational function in t. If the condition holds, then the offset to \mathcal{C} has two components, and both components are rational. In fact, these two components are parametrized as

$$\mathcal{P}(t) + \frac{d}{m(t)}\mathcal{N}(t)$$
, and $\mathcal{P}(t) - \frac{d}{m(t)}\mathcal{N}(t)$,

where $P_1^{'}(t)^2 + P_2^{'}(t)^2 = a(t)^2/b(t)^2$ and m(t) = a(t)/b(t).

If the rational Pythagorean hodograph condition does not hold, then the offset is irreducible and we may determine its rationality.

Example 11. We consider as initial curve the parabola of equation $y = x^2$, and its proper parametrization

$$\mathcal{P}(t) = (t, t^2).$$

The normal vector associated to $\mathcal{P}(t)$ is $\mathcal{N}(t) = (-2t, 1)$. Now, we check the rational Pythagorean hodograph condition

$$P_{1}^{'}(t)^{2} + P_{2}^{'}(t)^{2} = 4t^{2} + 1,$$

and we observe that $4t^2+1$ is not the square of a rational function. Therefore, the offset to the parabola is irreducible. In fact, the offset to the parabola, at a generic distance d, can be parametrized as

$$\left(\frac{(t^2+1-4dt)(t^2-1)}{4t\,(t^2+1)},\frac{t^6-t^4-t^2+1+32dt^3}{16t^2\,(t^2+1)}\right).$$

The implicit equation of the offset to the parabola is

$$-y^2 + 32x^2d^2y^2 - 8x^2yd^2 + d^2 + 20x^2d^2 - 32x^2y^2 + 8d^2y^2 + 2yx^2 - 8yd^2 + 48x^4d^2 - 16x^4y^2 - 48x^2d^4 + 40x^4y + 32x^2y^3 - 16d^4y^2 - 32d^4y + 32d^2y^3 - x^4 + 8d^4 + 8y^3 - 16x^6 + 16d^6 - 16y^4 = 0.$$

3

Computer Generated Progress in Lattice Paths Theory

Modern computer algebra is capable of contributing to contemporary research in various scientific areas. In this section, we present some striking success of computer algebra in the context of lattice paths theory, a theory belonging to the area of combinatorics. A lattice is something like the city map of Manhattan, a perfect grid where all streets go either north-south or east-west. A lattice path then corresponds to a possible way a person in Manhattan may take who wants to get from A to B.

Combinatorics deals with the enumeration (counting) of objects, and enumeration questions concerning lattice paths arise naturally: How many ways are there to get from A to B? How many of them avoid a third point C or an entire area of the city? How many go more often north than south? How many avoid visiting the same point twice? How many have an optimal length? Starting disoriented at A and randomly continuing the way at each street crossing, what is the probability of eventually reaching B? What is the expected length of such a random walk?

These and many other questions have been intensively studied already for several centuries. Some are completely answered since long, others are still wide open today. Lattice paths are studied not only for supporting tourists who got lost in the middle of New York, but they are also needed in a great number of physical applications. For example, the laws governing the diffusion of small molecules through a crystal grid depend on results from lattice paths theory.

Paths in the Quarter Plane 3.1

We consider lattice walks confined to a quarter plane. A quarter plane may be imagined as a chess board which at two of its four sides (say, the right and the upper side) is prolonged to infinity. The prolongation removes three of the chess board's corners, only its lower left corner remains. This corner is the starting point of our paths.

Let us imagine that there is a chess piece which is able to move a single step north (N), south (S), west (W), or east (E) at a time. Then, among all the possible paths that this chess piece can perform, we are interested in those where the chess piece ends up again at the board's corner, the starting point of the journey. The number of these paths depends, of course, on the number n of steps we are willing to make. With n=2 steps, there are only two possible paths: $(0,0) \xrightarrow{E} (1,0) \xrightarrow{W} (0,0)$ and $(0,0) \xrightarrow{N} (0,1) \xrightarrow{S} (0,0)$. For

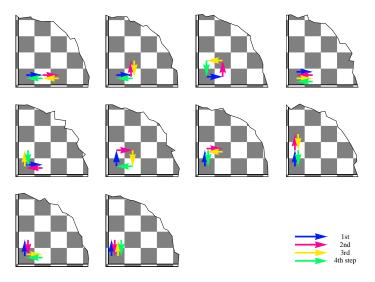


FIGURE 7 All closed Manhattan walks with four steps

n=3 steps, there are no such paths, and it is easy to see that there are no such paths whenever n is odd. For n=4 steps, there are ten paths, they are depicted in Figure 7. For n=40 steps, there are exactly as many as $160\,599\,522\,947\,154\,548\,400$ different paths.

That last number can obviously not be obtained by simply writing down all the possible paths. (Not even the fastest computer would be able to finish this task within our lifetime.) The number for n=40 was obtained by means of a formula which produces the number a_n of paths for any given number n of steps. According to this formula, we have

$$a_{2n} = \frac{2}{(n+1)(n+2)} {2n \choose n} {2n+1 \choose n}$$
 $(n \ge 0)$.

and $a_n = 0$ if n is odd. This is a classical result and it can in fact be proven by elementary means.

In order to fully understand the combinatorics of our chess piece, it is not sufficient to know the numbers a_n . For a complete knowledge, it is also necessary to know the number of paths that the chess piece can take starting from the corner (0,0) and ending at an arbitrary field (i,j). We can denote this number by $a_{n,i,j}$ and have, for example, $a_{40,6,4}=2\,482\,646\,858\,370\,896\,735\,656$ paths going in n=40 steps from the corner to the field in the 6th column and the 4th row.

It cannot be expected that there is a simple formula for $a_{n,i,j}$ as there is for $a_n = a_{n,0,0}$. In a sense, the numbers $a_{n,i,j}$ are "too complicated" to admit a formula. But among the sequences which do not have a simple formula, some are still more complicated than others. Combinatorialists have invented a hierarchy of classes for distinguishing different levels of "complicatedness". For a sequence $a_{n,i,j}$, they consider the formal infinite series

$$f(t, x, y) := \sum_{n=0}^{\infty} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{n,i,j} x^{i} y^{j} t^{n}.$$

This series is called *rational* or *algebraic* or *holonomic*, depending on whether it satisfies certain types of equations whose precise form need not concern us here. The only thing relevant for now is that these notions create a hierarchy

rational series \subseteq algebraic series \subseteq holonomic series \subseteq all series.

A modern research program initiated by Bousquet-Melou and Mishna [BM02, Mis07, BMM08] is the classification of all the series arising from the lattice paths in the quarter plane performed by chess pieces with different step sets than N, S, W, E.

Computer Algebra Support 3.2

Thanks to research undertaken recently by members of RISC (M. Kauers and C. Koutschan) in collaboration with A. Bostan (France) and D. Zeilberger (USA), we are now in the fortunate situation that the combinatorial analysis of lattice paths is completely automatized: there are computer programs which, given any set S of admissible steps drawn from $\{N, S, E, W, NW, NE, SW, SE\}$, produce a formula for the number of paths that a chess piece can do, if it starts in the corner, is only allowed to make steps from S, and wants to return to the corner after exactly n steps. Also for the more general problem of finding out to which class a series f(t, x, y) describing the full combinatorial nature of the chess piece belongs, there are computer programs available.

Unlike a traditional combinatorialist who would try to *derive* such formulas from known facts about lattice paths, the computer follows a paradigm that could be called *guess'n'prove*. This paradigm, which proves useful in many other combinatorial applications of computer algebra, can be divided into the following three steps:

1. Gather. For small values of n, compute the number a_n of paths with n steps by a direct calculation. For instance, for the step set N, S, W, E

taken as example above, a computer is able to find without too much effort that the sequence (a_{2n}) for $n = 0, 1, \ldots$ starts with the terms

2. Guess. Given the initial terms, the computer can next search for formulas matching them. More convenient than a direct search for closed form expressions is a search for recurrence equations matching the data, since this can be done by algorithms reminiscent of polynomial interpolation. Such algorithms are implemented in widely available software packages, for instance in a package by Mallinger implemented at RISC [Mal96b]. For the data from our example, this package "guesses" the recurrence equation

$$(n+2)(n+3)a_{2(n+1)} - 4(2n+1)(2n+3)a_{2n} = 0.$$

This equation is constructed such as to fit the first nine terms, but there is a priori no guarantee that it is valid, as we desire, for all n.

3. Prove. Experience says that an automatically guessed formula is always correct, but experience is not a formal proof. A formal proof can, however, also be constructed by the computer. We have an algorithm which takes as input a step set and a conjectured recurrence equation, and which outputs either a rigorous formal proof of the recurrence equation, or a counter example. The details of this algorithm are beyond the scope of this text.

There are only two possible reasons for which this guess'n'prove procedure may fail. The first is that for the particular step set at hand, the corresponding counting sequence does not satisfy any recurrence. In this case (which may indeed happen) the computer would indefinitely continue to search for a recurrence, because it is at present not possible to detect automatically that no recurrence exists. The second possible case of failure happens when a counting sequence satisfies only extremely huge recurrence equations (say, with millions of terms). In this case, although the computer would in principle be able to discover and to prove this recurrence, it may well be that in practice it is not, because the necessary computations are too voluminous to be completed by current computer architectures within a reasonable amount of time. The fact that such extremely large objects do actually arise induces a demand for faster algorithms in computer algebra. Such improved algorithms are therefore a natural subject of ongoing research.

3.3 Gessel's Conjecture

Let us now turn to a different imaginary chess piece. This new chess piece is able to move a single step left (E) or right (W), or diagonally a single step

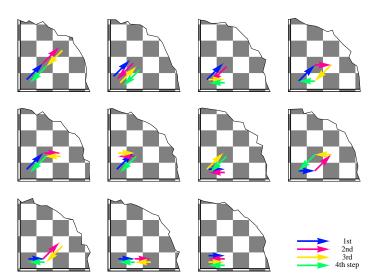
down-left (SE) or up-right (NW). We are interested again in the number of paths that take this chess piece from the corner of the (infinitely prolonged) chess board in n steps back to that corner. The counting sequence now starts as

As an example, the eleven paths consisting of four steps are depicted in Figure 8.

The lattice paths just described were first considered by Gessel and are now known as *Gessel walks*. Gessel observed that there appears to hold the formula

$$a_{2n} = 16^n \frac{\left(\frac{5}{6}\right)_n \left(\frac{1}{2}\right)_n}{\left(\frac{5}{3}\right)_n (2)_n} \qquad (n \ge 0),$$

where the notation $(x)_n$ stands for the product $x(x+1)(x+2)\cdots(x+n-1)$, a variation of the factorial function introduced by Pochhammer. Neither Gessel himself nor any other combinatorialist was, however, able to provide a rigorous proof of this formula. It became known as the Gessel conjecture and circulated as an open problem through the community for several years. Only in 2008, a proof was found at RISC by Kauers, Koutschan, and Zeilberger [KZ08, KKZ08]. Their proof relies on heavy algebraic computations that follow essentially the *quess'n'prove* paradigm described before.



The proof of Gessel's conjecture settles the nature of Gessel walks returning to the starting point. The nature of Gessel walks with arbitrary endpoint (i, j) is more difficult to obtain. This question was addressed by Bostan and Kauers [BK09a] after the proof of Gessel's original conjecture. By extensive algebraic calculations, they were able to prove that the series f(t, x, y) encoding the numbers $a_{n,i,j}$ of Gessel walks with n steps ending at (i,j) is algebraic. For at least two different reasons, this is a surprising result. First, it was not at all expected that f(t, x, y) is algebraic. Combinatorial intuition seemed to suggest that f(t, x, y) is perhaps holonomic, or not even that. Second, it was not to be expected that the intensive computations needed for establishing the algebraicity of f(t, x, y) were feasible for today's computers. As they were, the combinatorial nature of Gessel walks can now be considered as solved.

It is fair to say that the classification of the Gessel walks is the most difficult classification problem for lattice paths in the quarter plane. Indeed, all other kinds of paths can be classified by traditional means relying on group theory [BMM08]. Gessel's paths are famous partly because they are the only ones which appear to resist this group theoretic approach. This is why the clarification of their nature by means of computer algebra, as previously described, was highly appreciated by the community.

3.4 Lattice Paths in 3D

One of the advantages of a computer algebra approach to lattice paths classification is that computer programs, once written, can be easily adapted to related problems. Bostan and Kauers [BK08] applied their programs first developed for analyzing the Gessel paths to start a classification of lattice paths in a three dimensional lattice. In analogy to the problem considered before in 2D, lattice paths were considered which start in the corner of a space that extends to infinity in now three different directions, that space may be viewed as a distinguished octant of the usual Cartesian three dimensional space.

In addition to going north (N), south (S), east (E), or west (W), there are the additional directions up (U) and down (D). Also combined directions such as NE or SWU are possible. Basic steps are now more conveniently written as vectors, e.g., (1,-1,0) for NE or (-1,1,1) for SWU. While in 2D, there were eight basic steps (N, S, E, W, NE, NW, SE, SW), there are now 26 basic steps in 3D. For any subset \mathcal{S} of those, we can imagine a chess piece moving in 3D that is only allowed to take steps from \mathcal{S} , and we may ask how many paths it can take starting from the corner, making n steps, and ending again in the corner. For these numbers, call them again a_n , there may or may not be a simple formula. (Usually there is none.) If, more generally, the number of paths consisting of n steps and ending at a point (i, j, k) is denoted $a_{n,i,j,k}$, we can consider the infinite series

$$f(t, x, y, z) = \sum_{n=0}^{\infty} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} a_{n,i,j,k} x^{i} y^{j} z^{k} t^{n}$$

and may ask whether that series is rational, algebraic, holonomic, or non-holonomic. The answer will depend on the choice \mathcal{S} of admissible steps.

In Figure 9, some step sets S are depicted for which the corresponding series is algebraic, holonomic, or non-holonomic. For example, the first step set in the top row is

$$S = \{(-1, 1, 1), (0, -1, -1), (0, -1, 0), (1, 0, 0), (1, 0, 1)\}.$$

The distinguished octant to which the paths are restricted is the octant containing (1,1,1), which corresponds to the top-right-back corner in the diagrams of Figure 9. The counting sequence for paths returning to the corner with S as above starts

For example, the only possible path with three steps is

$$(0,0,0) \xrightarrow{(1,0,0)} (1,0,0) \xrightarrow{(-1,1,1)} (0,1,1) \xrightarrow{(0,-1,-1)} (0,0,0).$$

The interested reader may wish to determine the five possible paths with six steps. He or she will find that this is a much more laborious and error prone task than for planar lattice paths.

Most of the possible step sets S in 3D lead to series which are not holonomic, only a fraction of them is holonomic or even algebraic. Out of those, the examples depicted in Figure 9 were chosen such as to illustrate that the position of a step set in the hierarchy is not necessarily related to what might be expected intuitively from the geometric complexity of the step set. For example, the first step set in the third row looks rather regular, yet the corresponding series is not holonomic. On the other hand, the third step set of the first row looks rather irregular, yet the corresponding series is algebraic.

Computer algebra was used in the discovery of these phenomena. The next challenging task is to explain them. As we have seen for Gessel's walks, computer algebra is ready to contribute also in these investigations. It will, in general, be of increasing importance the more the theory advances towards objects that are beyond the capabilities of traditional hand calculations.

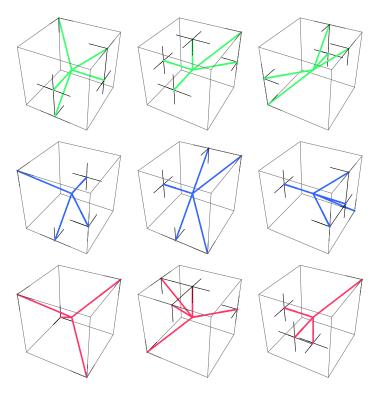


FIGURE 9 Some step sets for lattice walks in 3D whose counting sequences appear to be algebraic (first row), holonomic but not algebraic (second row), or not holonomic (third row).

4 Symbolic Summation in Particle Physics

Mathematical algorithms in the area of symbolic summation have been intensively developed at RISC in the last 15 years, see e.g., [PS95b, Mal96b, Weg97, PR97, PS03, M06]. Meanwhile they are heavily used by scientists in practical problem solving.

We present in this section a brand new interdisciplinary project in which we try to deal with challenging problems in the field of particle physics and perturbative quantum field theory with the help of our summation technology. Generally speaking, the overall goal in particle physics is to study the basic elements of matter and the forces acting among them. The interaction of these particles can be described by the so called Feynman diagrams, respectively Feynman integrals. Then the crucial task is the concrete evaluation

of these usually rather difficult integrals. In this way, one tries to obtain additional insight how, e.g., the fundamental laws control the physical universe.

In cooperation with the combinatorics group (Peter Paule) at RISC and the theory group (Johannes Blümlein) at Deutsches Elektronen-Synchrotron (DESY Zeuthen, a research centre of the German Helmholtz association), we are in the process of developing flexible and efficient summation and special function algorithms that assist in this task, i.e., simplification, verification and manipulation of Feynman integrals and sums, and of related expressions. As it turns out, the software package Sigma [Sch07] plays one of the key roles: it is able to simplify highly complex summation expressions that typically arise within the evaluation of such Feynman integrals; see [BBKS07, MS07, BBKS08, BKKS09a, BKKS09b].

From Feynman diagrams to symbolic summation

Figure 10

After sketching the basic summation tools that are used in such computations, we present two examples popping up at the scientific front of particle physics.

The Underlying Summation Principles 4.1

The summation principles of telescoping, creative telescoping and recurrence solving for hypergeometric terms, see e.g. [PWZ96], can be considered as the breakthrough in symbolic summation. Recently, these principles have been generalized in Sigma from single nested summation to multi-summation by exploiting a summation theory based on difference fields [Kar81, Sch05,

Sch08, Sch09]. As worked out, e.g., in [BBKS07], these methods can help to solve problems from particle physics.

Specification (Indefinite summation by telescoping). Given an indefinite sum $S(a) = \sum_{k=0}^{a} f(k)$, find g(j) such that

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

holds within the summation range $0 \le j \le a$. Then by telescoping, one gets

$$S(a) = g(a+1) - g(0).$$

Example. For the sum expression

$$f(j) = \frac{(2j+k+N+2)j!k!(j+k+N)!}{(j+k+1)(j+N+1)(j+k+1)!(j+N+1)!(k+N+1)!} + \frac{j!k!(j+k+N)!(-S_1(j)+S_1(j+k)+S_1(j+N)-S_1(j+k+N))}{(j+k+1)!(j+N+1)!(k+N+1)!}$$
(2)

involving the single harmonic sums defined by $S_1(j) := \sum_{i=1}^j \frac{1}{i}$ Sigma computes the solution

$$g(j) = \frac{(j+k+1)(j+N+1)j!k!(j+k+N)!\left(S_1(j)-S_1(j+k)-S_1(j+N)+S_1(j+k+N)\right)}{kN(j+k+1)!(j+N+1)!(k+N+1)!}$$
(3)

of (1); note that the reader can easily verify the correctness of this result by plugging in (2) and (3) into (1) and carrying out simple polynomial arithmetic in combination with relations such as $S_1(j+1) = S_1(j) + \frac{1}{j+1}$ and (j+1)! = (j+1)j!. Therefore summing (1) over j yields (together with a proof)

$$\sum_{j=0}^{a} f(j) = \frac{S_1(k) + S_1(N) - S_1(k+N)}{kN(k+N+1)N!} + \frac{(2a+k+N+2)a!k!(a+k+N)!}{(a+k+1)(a+N+1)(a+k+1)!(a+k+1)!(k+N+1)!} + \frac{(a+1)!k!(a+k+N+1)!(S_1(a) - S_1(a+k) - S_1(a+N) + S_1(a+k+N))!}{kN(a+k+1)!(a+N+1)!(a+N+1)!}.$$

In other words, we obtained the following simplification: the double sum $\sum_{j=0}^{a} f(j)$ with (2) could be simplified to an expression in terms of single harmonic sums. Later we shall reuse this result by performing the limit $a \to \infty$:

$$\sum_{j=0}^{\infty} f(j) = \lim_{a \to \infty} \sum_{j=0}^{a} f(j) = \frac{S_1(k) + S_1(N) - S_1(k+N)}{kN(k+N+1)N!}.$$
 (4)

In most cases this telescoping trick fails, i.e., such a solution g(j) for (1) does not exist. If the summand f(j) depends on an extra discrete parameter, say N, one can proceed differently with Zeilberger's creative telescoping paradigm.

Specification (Deriving Recurrences by Creative Telescoping). Given an integer d>0 and given a sum

$$S(a, N) := \sum_{j=0}^{a} f(N, j)$$
 (5)

with an extra parameter N, find constants $c_0(N), \ldots, c_d(N)$, free of j, and g(N,j) such that for $0 \le j \le a$ the following summand recurrence holds:

$$c_0(N)f(N,j) + \dots, c_d(N)f(N+d,j) = g(N,j+1) - g(N,j).$$
 (6)

If one succeeds in this task, one gets by telescoping the recurrence relation

$$c_0(N)S(a, N) + \cdots + c_d(N)S(a, N+d) = g(N, a+1) - g(N, 0).$$

Example. For d=1 and the summand

$$f(N,j) = \frac{S_1(j) + S_1(N) - S_1(j+N)}{jN(j+N+1)N!}$$

Sigma computes the solution $c_0(N) = -N(N+1)^2$, $c_1(N)(N+1)^3(N+2)$, and

$$g(N,j) = \frac{jS(1,j) + (-N-1)S(1,N) - jS(1,j+N) - 2}{(j+N+1)N!}$$

of (6); again the reader can easily verify the correctness of this computation by simple polynomial arithmetic. Hence, summing (6) over $1 \le j \le a$ gives

$$-NS(N,a) + (1+N)(2+N)S(N+1,a) = \frac{a(a+1)}{(N+1)^3(a+N+1)(a+N+2)N!} + \frac{(a+1)(S_1(a) + S_1(N) - S_1(a+N))}{(N+1)^2(a+N+2)N!}$$
(7)

for the sum (5). Later we need the following additional observation: the limit

$$S'(N) := \lim_{a \to \infty} S(N, a) = \sum_{j=0}^{\infty} \frac{S_1(j) + S_1(N) - S_1(j+N)}{jN(j+N+1)N!}$$
(8)

exists; moreover, it is easy to see that the right hand side of (7) tends in the limit $a \to \infty$ to $\frac{(N+1)S_1(N)+1}{(N+1)^3N!}$. In other words, the infinite series (8) satisfies the recurrence

$$-NS'(N) + (1+N)(2+N)S'(N+1) = \frac{(N+1)S_1(N) + 1}{(N+1)^3 N!}.$$
 (9)

Summarizing, with creative telescoping one can look for a recurrence of the form

$$a_0(N)S(N) + \dots + a_1(N)S(N+d) = q(N).$$
 (10)

Finally, Sigma provides the possibility to solve such recurrence relations in terms of indefinite nested sums and products.

Example. We use Sigma's recurrence solver and compute the general solution

$$\frac{1}{N(N+1)N!}c + \frac{S_1(N)^2 + S_2(N)}{2N(N+1)N!}$$

for a constant c of the recurrence (9). Checking the initial value $S'(1) = \frac{1}{2}$ (this evaluation can be done again by using, e.g., the package Sigma) determines c = 0, i.e., we arrive at

$$S'(N) = \sum_{j=1}^{\infty} \frac{S_1(j) + S_1(N) - S_1(j+N)}{jN(j+N+1)N!} = \frac{S_1(N)^2 + S_2(N)}{2N(N+1)!}.$$
 (11)

More generally, we can handle with Sigma the following problem.

Specification (Recurrence solving). Given a recurrence of the form (10), find all solutions in terms of indefinite nested sum and product expressions (also called d'Alembertian solution).

Based on the underlying algorithms, see e.g. [AP94, BKKS09a], the derived d'Alembertian solutions of (10) are highly nested: in worst case the sums will reach the nesting depth r-1. In order to simplify these solutions (e.g., reducing the nesting depth), a refined telescoping paradigm is activated. For an illuminative example see Section 4.3.

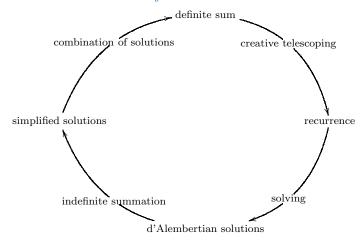
One can summarize this interplay of the different summation principles in the "summation spiral" [Sch04] illustrated in Figure 11.

4.2 Example 1: Simplification of Multi-Sums

The first example is part of the calculation of the so called polarized and unpolarized massive operator matrix elements for heavy flavor production [BBK06, BBK07]. Here two–loop Feynman integrals arise which can be reformulated in terms of double infinite series by skillful application of Mellin-Barnes integral representations. One of the challenging sums [BBK06] in this context is

$$S(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \underbrace{\frac{\varepsilon^{-\varepsilon\gamma}}{\Gamma(\varepsilon+1)} \left(\frac{\Gamma(k+1)}{\Gamma(k+2+N)} \frac{\Gamma(\frac{\varepsilon}{2})\Gamma(1-\frac{\varepsilon}{2})\Gamma(j+1-\frac{\varepsilon}{2})\Gamma(j+1+\frac{\varepsilon}{2})\Gamma(k+j+1+N)}{\Gamma(j+1-\frac{\varepsilon}{2})\Gamma(j+2+N)\Gamma(k+j+2)} + \frac{\Gamma(k+1)}{\Gamma(k+2+N)} \frac{\Gamma(-\frac{\varepsilon}{2})\Gamma(1+\frac{\varepsilon}{2})\Gamma(j+1+\varepsilon)\Gamma(j+1-\frac{\varepsilon}{2})\Gamma(k+j+1+\frac{\varepsilon}{2}+N)}{\Gamma(j+1)\Gamma(j+2+\frac{\varepsilon}{2}+N)\Gamma(k+j+2+\frac{\varepsilon}{2})} \right);$$

$$(12)$$



The Sigma-summation spiral

Figure 11

here N is an integer variable and $\Gamma(x)$ denotes the gamma function, see e.g. [AAR00], which evaluates to $\Gamma(k) = (k-1)!$ for positive integers k.

Remark. Usually, Feynman integrals (and sums obtained, e.g., by Mellin Barnes representations) cannot be formalized at the space-time dimension D=4. One overcomes this problem by an analytic continuation of the space-time $D=4+\varepsilon$ for a small parameter ε . Then one can extract the needed information by calculating sufficiently many coefficients of the Laurent-series expansion about $\varepsilon=0$.

For instance, in our concrete sum (12) one is interested in the first coefficients $F_0(N), F_1(N), F_2(N), \ldots$ in the expansion

$$S(N,\varepsilon) = F_0(N) + F_1(N)\varepsilon + F_2(N)\varepsilon^2 + \dots$$
 (13)

In order to get these components, we proceed as follows. First, we compute, as much as needed, the coefficients $f_0(N, k, j), f_1(N, k, j), \ldots$ of the series expansion

$$f(N,k,j,\varepsilon) = f_0(N,k,j) + f_1(N,k,j)\varepsilon + f_1(N,k,j)\varepsilon^2 + f_1(N,k,j)\varepsilon^2 + \dots$$
(14)

on the summand level. Then, it follows (by convergence arguments) that for all $i \geq 0$,

$$F_i(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} f_i(N, k, j).$$

Remark. The gamma function $\Gamma(x)$ is analytic everywhere except at the points $x=0,-1,-2,\ldots$, and there exist formulas that relate, e.g., the deriva-

tive of the gamma function $\Gamma(x+k)$ w.r.t. x with the sums $S_a(k) = \sum_{i=1}^k \frac{1}{i^a}$ for positive integers a.

Due to such formulas, one can compute straightforwardly the first coefficients $f_i(N,k,j)$ in (14) for the explicitly given summand in (12). E.g., $f_0(N,k,j)$ is nothing else than (2). Thus the constant term $F_0(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} f_0(N,k,j)$ in (13) is given by

$$F_{0}(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+N+2)j!k!(j+k+N)!}{(j+k+1)(j+N+1)!(j+N+1)!(k+N+1)!} + \frac{j!k!(j+k+N)!(-S_{1}(j)+S_{1}(j+k)+S_{1}(j+N)-S_{1}(j+k+N))}{(j+k+1)!(j+N+1)!(k+N+1)!} \right).$$

$$(15)$$

We are faced now with the problem to simplify (15), so that it can be processed further in particle physics. Exactly at that point we are in business with our summation tools from Section 4.1. First observe that the inner sum of (15) is equal to the right hand side of (4). Hence with (11) we find that

$$\sum_{k=1}^{\infty} \sum_{i=0}^{\infty} f_i(N, k, j) = \frac{S_1(N)^2 + S_2(N)}{2N(N+1)!}.$$

Finally, we add the missing term $\sum_{j=0}^{\infty} f_i(N,0,j) = \frac{S_2(N)}{N(N+1)!}$ (derived by the same methods as above). To sum up, we simplified the expression (15) to

$$F_0(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} f_0(N, k, j) = \frac{S_1(N)^2 + 3S_2(N)}{2N(N+1)!}.$$

In [BBK06] the authors derived this constant term and also the linear term

$$F_1(N) = \frac{-S_1(N)^3 - 3S_2(N)S_1(N) - 8S_3(N)}{6N(N+1)!}$$

in (13) by skillful application of suitable integral representations.

Contrary, our computations can be carried out purely mechanically with the computer. Essentially, this enables us to compute further coefficients in (13) by just pressing a button (and having some coffee in the meantime):

$$F_{2}(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} f_{2}(N, k, j) = \frac{1}{96N(N+1)!} \left(S_{1}(N)^{4} + (12\zeta_{2} + 54S_{2}(N))S_{1}(N)^{2} + 104S_{3}(N)S_{1}(N) - 48S_{2,1}(N)S_{1}(N) + 51S_{2}(N)^{2} + 36\zeta_{2}S_{2}(N) + 126S_{4}(N) - 48S_{3,1}(N) - 96S_{1,1,2}(N) \right),$$

$$F_{3}(N) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} f_{3}(N, k, j) = \frac{1}{960N(N+1)!} \left(S_{1}(N)^{5} + (20\zeta_{2} + 130S_{2}(N))S_{1}(N)^{3} + (40\zeta_{3} + 380S_{3}(N))S_{1}(N)^{2} + (135S_{2}(N)^{2} + 60\zeta_{2}S_{2}(N) + 510S_{4}(N))S_{1}(N) - 240S_{1,1,3}(N) - 240S_{4,1}(N) - 240S_{3,1}(N)S_{1}(N) - 240S_{1,1,2}(N)S_{1}(N)$$

+
$$160\zeta_2 S_3(N) + S_2(N)(120\zeta_3 + 380S_3(N)) + 624S_5(N)$$

+ $(-120S_1(N)^2 - 120S_2(N)) S_{2,1}(N) + 240S_{2,2,1}(N));$

here $\zeta_r = \sum_{i=1}^{\infty} \frac{1}{i^r}$ denote the zeta-values at r and the harmonic sums [BK99, Ver99] for nonzero integers r_1, \ldots, r_n are defined by

$$S_{r_1,\dots,r_n}(N) = \sum_{k_1=1}^{N} \frac{\operatorname{sign}(r_1)^{k_1}}{k^{|r_1|}} \sum_{k_2=1}^{k_1} \frac{\operatorname{sign}(r_{m-1})^{k_2}}{k_2^{|r_1|}} \cdots \sum_{k_r=1}^{k_{r-1}} \frac{\operatorname{sign}(r_n)^{k_r}}{k_r^{|r_1|}}.$$
(16)

E.g., we find the linear coefficient $F_1(N)$ in 30 seconds, the quadratic coefficient $F_2(N)$ in 4 minutes and the cubic coefficient $F_3(N)$ in less than one hour.

Example 2: Solving Large Recurrence Relations 4.3

One of the hardest problem that has been considered in the context of Feynman integrals is the calculation of the symbolic Mellin-moments of the unpolarized 3–loop splitting functions and Wilson coefficients for deep—inelastic scattering [MVV04, VMV04, VVM05]: several CPU years were needed for this job. In order to get these results, specialized and extremely efficient software [Ver99] have been developed. Based on deep insight and knowledge of the underlying physical problem fine tuned ansatzes for the computations have been used in addition.

In a recent attempt [BKKS09a, BKKS09b] we explored a different, rather flexible ansatz in order to determine such coefficients. We illustrate this approach for the $C_F N_F^2$ -term, say $F(N) = P_{gq,2}(N)$, of the unpolarized 3-loop splitting function; see [BKKS09b, Exp. 1]. Namely, we start with the initial values F(i) for i = 3, ..., 112 where the first ones are given by

$$\frac{1267}{648}, \frac{54731}{40500}, \frac{20729}{20250}, \frac{2833459}{3472875}, \frac{29853949}{44452800}, \frac{339184373}{600112800}, \frac{207205351}{428652000}, \frac{152267426}{363862125}, \dots$$

Then given this data, one can establish (within 7 seconds) by Manuel Kauers' very efficient recurrence guesser (see also Section 3.2) the following recurrence:

$$(1-N)N(N+1)(N^6+15N^5+109N^4+485N^3+1358N^2+2216N+1616)F(N)$$

$$+N(N+1)(3N^7+48N^6+366N^5+1740N^4+5527N^3+11576N^2+14652N+8592)F(N+1)$$

$$-(N+1)(3N^8+54N^7+457N^6+2441N^5+9064N^4+23613N^3$$

$$+41180N^2+43172N+20768)F(N+2)$$

$$+(N+4)^3(N^6+9N^5+49N^4+179N^3+422N^2+588N+368)F(N+3)=0.$$

We remark that in principle this guess might be wrong, but by rough estimates this unlucky case occurs with probability of about 10^{-65} (if we do not trust in this result, we should not trust any computation: e.g., undetectable hardware errors have a much higher chance to happen).

Given this recurrence, we apply the recurrence solver of Sigma: internally, one succeeds in factorizing the recurrence into linear right hand factors; see [BKKS09b, Exp. 1]. As a consequence, Sigma finds (within 3 seconds) the solution

$$F(N) = -\frac{32}{9} \frac{N^2 + N + 2}{(N-1)N(N+1)} + \frac{64}{9} \frac{\left(N^2 + N + 2\right) \sum_{i=1}^{N} \frac{i^4 + 7i^2 + 4i + 4}{(i+1)(i^2 - i + 2)(i^2 + i + 2)}}{(N-1)N(N+1)}$$
$$-\frac{8}{3} \frac{\left(N^2 + N + 2\right) \sum_{i=1}^{N} \frac{\left(i^4 + 7i^2 + 4i + 4\right) \sum_{j=1}^{i} \frac{\left(j^2 - j + 2\right) \left(j^6 - 3j^5 + 19j^4 - 13j^3 + 44j^2 + 8j + 8\right)}{(j+1)(j^4 + 7j^2 + 4j + 4)(j^4 - 4j^3 + 13j^2 - 14j + 8)}}{(i+1)(i^2 - i + 2)(i^2 + i + 2)}}{(N-1)N(N+1)}.$$

Next, we activate our sum simplifier (based on refined telescoping [Sch08]) and end up at the closed form

$$F(N) = -\frac{4(N^2 + N + 2)}{3(N - 1)N(N + 1)}S_1(N)^2 + \frac{8(8N^3 + 13N^2 + 27N + 16)}{9(N - 1)N(N + 1)^2}S_1(N)$$
$$-\frac{8(4N^4 + 4N^3 + 23N^2 + 25N + 8)}{9(N - 1)N(N + 1)^3} - \frac{4(N^2 + N + 2)}{3(N - 1)N(N + 1)}S_2(N)$$

in terms of the harmonic sums given by (16). At this point we make the following remark: we are not aware of the existence of any other software that can produce this solution of the rather simple recurrence given above. Summarizing, we determined the $C_F N_F^2$ -term of the unpolarized 3-loop splitting function $F(N) = P_{gq,2}(N)$ by using its first 110 initial values without any additional intrinsic knowledge.

In order to get an impression of the underlying complexity, we summarize the hardest problem. For the most complicated expression (the C_F^3 -contribution to the unpolarized 3-loop Wilson coefficient for deeply inelastic scattering, see [BKKS09b, Exp. 6]) M. Kauers could establish a recurrence of order 35 within 20 days and 10Gb of memory by using 5022 such initial values; note that the found recurrence has minimal order and uses 32MB of memory size. Then Sigma used 3Gb of memory and around 8 days in order to derive the closed form of the corresponding Wilson coefficient. The output fills several pages and consists of 30 (algebraically independent) harmonic sums (16), like e.g.,

$$S_{-3,1,1,1}, S_{2,2,1,1}, S_{-2,-2,1,1}, S_{2,-2,1,1}, S_{-2,2,1,1}, S_{-2,1,1,2}, S_{2,1,1,1,1}, S_{-2,1,1,1,1}.$$

In total, we used 4 month of computation time in order to treat all the problems from [MVV04, VMV04, VVM05].

These results from [BKKS09a, BKKS09b] illustrate that one can solve 3-loop integral problems efficiently by recurrence guessing and recurrence solving under the assumptions that sufficiently many initial values (in our case maximally 5022) are known. In order to apply our methods to such problems, methods at far lower expenses have to be developed that can produce this huge amount of initial values. This is not possible in the current state of art.

By concluding, in ongoing research we will try to combine the different ideas presented in Section 4 to find new, flexible and efficient methods that will take us one step further to evaluate automatically non-trivial Feynman integrals.

Nonlinear Resonance Analysis 5

In recent years (2004-2009) a new area of mathematical physics – Nonlinear Resonance Analysis (NRA) – has been developed at RISC. Its theoretical background was outlined in 1998, see [Kar98]. But the way to real-world applications was still long. In particular, appropriate calculation techniques and mathematical model fitting to physical systems had to be worked out. This has been achieved under the projects SBF-013 (FWF), ALISA (OeAD, Grant Nr.10/2006-RU), DIRNOW (FWF, P20164000), and CEN-REC (OeAD, Grant Nr.UA 04/2009). The main points of this work are briefly presented below.

What is resonance? 5.1

Physical examples

The phenomena of resonance has been first described and investigated by Galileo Galilei in 1638 who was fascinating by the fact that by "simply blowing" one can confer considerable motion upon even a heavy pendulum. A well-known example with Tacoma Narrows Bridge shows how disastrous resonances can be: on the morning of November 7, 1940, at 10:00 the bridge began to oscillate dangerously up and down, and collapsed in about 40 minutes. The experiments of Tesla [Che93] with vibrations of an iron column yielded in 1898 sort of a small earthquake in his neighborhood in Manhat-

tan, with smashed windows, swayed buildings, and panicky people in the streets.

Nowadays it is well-known fact that resonance is a common thread which runs through almost every branch of physics and technics, without resonance we wouldn't have radio, television, music, etc. Whereas linear resonances are studied quite good, their nonlinear counterpart was till recently Terra Incognita, out of the reach of any general theoretical approach. And this is though nonlinear resonances are ubiquitous in physics. Euler equations, regarded with various boundary conditions and specific values of some parameters, describe an enormous number of nonlinear dispersive wave systems (capillary waves, surface water waves, atmospheric planetary waves, drift waves in plasma, etc.) all possessing nonlinear resonances [ZLF92]. Nonlinear resonances appear in a great amount of typical mechanical systems [KM06]. Nonlinear resonance is the dominant mechanism behind outer ionization and energy absorption in near infrared laser-driven rare-gas or metal clusters [KB05]. Nonlinear resonance jump can cause severe damage to the mechanical, hydraulic and electrical systems [HMK03]. The characteristic resonant frequencies observed in accretion disks allow astronomers to determine whether the object is a black hole, a neutron star, or a quark star [W.K06]. The variations of the helium dielectric permittivity in superconductors are due to nonlinear resonances [KLPG04]. Temporal processing in the central auditory nervous system analyzes sounds using networks of nonlinear neural resonators [AJLT05]. The nonlinear resonant response of biological tissue to the action of an electromagnetic field is used to investigate cases of suspected disease or cancer [VMM05], etc.

Mathematical formulation

Mathematically, a resonance is an unbounded solution of a differential equation. The very special role of resonant solutions of nonlinear ordinary differential equations (ODEs) has been first investigated by Poincaré [Arn83] who proved that if a nonlinear ODE has no resonances, then it can be linearized by an invertible change of variables. Otherwise, only resonant terms are important, all other terms have the next order of smallness and can be ignored. In the middle of the 20th century, Poincaré's approach has been generalized to the case of nonlinear partial differential equations (PDEs) yielding what is nowadays known as KAM-theory (KAM for Kolmogorov-Arnold-Moser), [Kuk04]. This theory allows us to transform a nonlinear dispersive PDE into a Hamiltonian equation of motion in Fourier space [ZLF92],

$$i\,\dot{a}_{\mathbf{k}} = \partial \mathcal{H}/\partial a_{\mathbf{k}}^*,$$
 (17)

where $a_{\mathbf{k}}$ is the amplitude of the Fourier mode corresponding to the wavevector \mathbf{k} , $\mathbf{k} = (m, n)$ or $\mathbf{k} = (m, n, l)$ with integer m, n, l. The Hamiltonian \mathcal{H} is represented as an expansion in powers \mathcal{H}_i which are proportional to the

product of j amplitudes $a_{\mathbf{k}}$. For the simplicity of presentation, all the methods and results below are outlined for the case of non-zero cubic Hamiltonian \mathcal{H}_3 and 2-dimensional wavevector $\mathbf{k} = (m, n)$. A cubic Hamiltonian \mathcal{H}_3 has the form

$$\mathcal{H}_3 = \sum_{\mathbf{k_1, k_2, k_3}} V_{23}^1 a_1^* a_2 a_3 \delta_{23}^1 + \text{ complex conj.},$$

where for brevity we introduced the notation $a_j \equiv a_{\mathbf{k}_j}$ and $\delta_{23}^1 \equiv \delta(\mathbf{k_1} - \mathbf{k_2} - \mathbf{k_3})$ is the Kronecker symbol. If $\mathcal{H}_3 \neq 0$, three-wave process is dominant and the main contribution to the nonlinear evolution comes from the waves satisfying the following resonance conditions:

$$\omega(\mathbf{k}_1) + \omega(\mathbf{k}_2) - \omega(\mathbf{k}_3) = 0, \quad \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 = 0, \tag{18}$$

where $\omega(\mathbf{k})$ is a dispersion relation for the linear wave frequency. Corresponding dynamical equation yields the three-wave equation:

$$i\frac{da_{\mathbf{k}}}{dt} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \left[\frac{1}{2} V_{12}^{\mathbf{k}} a_1 a_2 \Delta_{12}^{\mathbf{k}} + V_{\mathbf{k}2}^{1*} a_1 a_2^* \Delta_{\mathbf{k}2}^{1} \right]. \tag{19}$$

The Hamiltonian formulation allows us to study the problems of various nature by the same method: all the difference between the problems of climate variability, cancer diagnostics and broken bridges is hidden in the form of the coefficients of the Hamiltonian, i.e. $V_{12}^{\mathbf{k}}$ and $V_{\mathbf{k}2}^{1*}$.

Kinematics and Dynamics 5.2

To compute nonlinear resonances in a PDE with given boundary conditions, one has to find linear eigenmodes and dispersion function $\omega = \omega(m, n)$, and rewrite the PDE in Hamiltonian form by standard methods (e.g. [Arn83], [ZLF92]). Afterwards two seemingly simple steps have to be performed.

- Step 1: To solve the algebraic Sys. (18) in integers and compute the coefficients V₁₂^k (they depend on the solutions of the Sys. (18)). This part of the NRA is called Kinematics.
- Step 2: To solve the Sys. (19), consisting of nonlinear ODEs; this part of the theory is called *Dynamics*.

In order to show mathematical and computational problems appearing on this way, let us regard one example. Let dispersion function have the form $\omega = 1/\sqrt{m^2 + n^2}$ (oceanic planetary waves) and regard a small domain of wavevectors, say $m, n \leq 50$. The first equation of Sys. (18) reads

$$(m_1^2 + n_1^2)^{-1/2} + (m_2^2 + n_2^2)^{-1/2} = (m_3^2 + n_3^2)^{-1/2}, (20)$$

the only standard way would be to get rid of radicals and solve numerically the resulting Diophantine equation of degree 8 in 6 variables:

$$(m_3^2 + n_3^2)^2 (m_1^2 + n_1^2) (m_2^2 + n_2^2) = \left[(m_1^2 + n_1^2) (m_2^2 + n_2^2) - (m_2^2 + n_2^2) (m_3^2 + n_3^2) - (m_1^2 + n_1^2) (m_3^2 + n_3^2) \right]^2$$
(21)

This means that at Step 1 we will need operate with integers of the order of $(50)^8 \sim 4 \cdot 10^{13}$. This means also that in physically relevant domains, with $m, n \leq 1000$, there is no chance to find solutions this way, using the present computers. At Step 2 we have $50 \times 50 = 2500$ complex variables $a_j, a_j^*, j = 1, 2, ..., 50$; correspondingly Sys. (19) consists of 2500 interconnected nonlinear ODEs. This being a dead-end, a search for novel computational methods is unavoidable.

Kinematics

Two main achievements in this part of our research are 1) The q-class method, and 2) Topological representation of resonance dynamics which we briefly present below.

The q-class method. Theoretical results of [Kar98] have been the basis for the development of a fast computational algorithm to compute nonlinear resonances outlined in [Kar06]. Various modifications of the q-class method have been implemented numerically ([KK06, KK07]) and symbolically ([KM07, KRF+07]) for a wide class of physically relevant dispersion functions. The efficiency of our method can be demonstrated by following example. Direct computation has been performed in 2005 by the group of Prof. S. Nazarenko (Warwick Mathematical School, UK) with dispersion function $\omega = (m^2 + n^2)^{1/4}$ for the case of 4-term resonance. For spectral domain $m, n \leq 128$, these computations took 3 days with Pentium 4; the same problem in the spectral domain $m, n \leq 1000$, is solved by the q-class method with Pentium 3 in 4.5 minutes.

We illustrate how the q-class method works, taking again Eq. (20) as an example. Two simple observations, based on school mathematics, can be made. First, for arbitrary integers m, n, the presentation

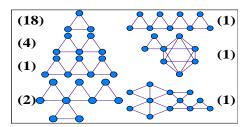
$$\sqrt{m^2 + n^2} = p\sqrt{q}$$

with integer p and square-free q is unique. Second, Eq. (20) has integer solutions only if in all three presentations

$$\sqrt{m_1^2 + n_1^2} = p_1 \sqrt{q_1}, \ \sqrt{m_2^2 + n_2^2} = p_2 \sqrt{q_2}, \ \sqrt{m_3^2 + n_3^2} = p_3 \sqrt{q_3}$$
 (22)

the irrationalities q_1, q_2, q_3 are equal, i.e. $q_1 = q_2 = q_3 = q$. This is only a necessary condition, of course. The number q is called index of a q-class, all pairs of integers (m, n) can be divided into disjoint classes by the index and search for solutions is perfored within each class separately. For each class, Eq. (20) takes a very simple form, $p_1^{-1} + p_2^{-1} = p_3^{-1}$, and can be solved in no time even with a simple calculator.

The general idea of the q-class method is, to use linear independence of some functions over the field of rational numbers \mathbb{Q} and can be generalized to much more complicated dispersion functions, e.g. $\omega = m \tanh \sqrt{m_1^2 + n_1^2}$. Though this approach does not work with rational dispersion functions, substantial computational shortcuts have also been found for this case ([KK07]).



Example of topological structure, spectral domain $|k_i| \leq 50$, each blue vertex corresponds to a pair (m,n) and three vertices are connected by arcs, if they constitute a resonant triad. The number in brackets shows how many times the corresponding cluster appears in the given spectral domain.

Figure 12

Topological representation of resonance dynamics. The classical representation of resonance dynamics by resonance curves [LHG67] is insufficient for two reasons. First, one has to fix a certain wavevector (m, n) and therefore this representation can not be performed generally. Second, no general method exists for finding integer points on a resonance curve. We have introduced a novel representation of resonances via a graph with vertices belonging to a subset of a two-dimensional integer grid. We have also proved that there exists a one-to-one correspondence between connected components of this graph and dynamical systems, subsystems of Sys. (19).

The topology for the example above is shown in the Figure 12; the dynamical system for the graph component (called *resonance cluster* in physics) consisting of 4 connected resonant triads (Figure 12, bottom left) reads (in real variables)

$$\begin{cases} \dot{a}_{1} = \alpha_{1}a_{2}a_{9}, & \dot{a}_{2} = \alpha_{2}a_{1}a_{9}, & \dot{a}_{3} = \alpha_{4}a_{4}a_{9}, & \dot{a}_{4} = \alpha_{5}a_{3}a_{9}, \\ \dot{a}_{5} = \alpha_{7}a_{8}a_{9}, & \dot{a}_{6} = \alpha_{10}a_{7}a_{8}, & \dot{a}_{7} = \alpha_{11}a_{6}a_{8}, \\ \dot{a}_{8} = \alpha_{12}a_{6}a_{7} + \alpha_{8}a_{5}a_{9}, & \dot{a}_{9} = \alpha_{3}a_{1}a_{2} + \alpha_{6}a_{3}a_{4} + \alpha_{9}a_{5}a_{8}. \end{cases}$$

$$(23)$$

Already this novel representation, both very simple and very informative, has attracted the attention of the peers of the Wolfram Demonstrations Project, and we have been invited to participate in the project¹.

Dynamics

Two main achievements in this part of our research are 1) explicit computation of *dynamical invariants*, [BK09b]; and 2) realization that *dynamical phase* is a parameter of the utmost importance in resonance dynamics [BK09c].

Dynamical invariant. In [KL08] it was shown that the dynamics of bigger clusters often can be reduced to the dynamics of smaller clusters, consisting of one or two triads only. Integrability of a triad, with dynamical system

$$\dot{a}_1 = Z a_2^* a_3, \quad \dot{a}_2 = Z a_1^* a_3, \quad \dot{a}_3 = -Z a_1 a_2,$$
 (24)

is a well known fact ([Whi90, LH04]), and its solution, simplified for the case of zero dynamical phase, reads

$$\begin{cases}
C_1(t) = \operatorname{dn}((-t+t_0) \ z \sqrt{I_{13}}, \frac{I_{23}}{I_{13}}) \sqrt{I_{13}} \\
C_2(t) = \operatorname{cn}((-t+t_0) \ z \sqrt{I_{13}}, \frac{I_{23}}{I_{13}}) \sqrt{I_{23}} \\
C_3(t) = \operatorname{sn}((-t+t_0) \ z \sqrt{I_{13}}, \frac{I_{23}}{I_{13}}) \sqrt{I_{23}}
\end{cases}$$
(25)

Here C_j , j=1,2,3 are real amplitudes within the standard representation $a_j=C_j\exp(i\theta_j)$, and t_o,I_{13},I_{23} are defined by initial conditions. The novelty of our approach lies in that we show ([BK09b]) that this system as a whole can be generally described by one time-dependent dynamical invariant of the form:

$$S_0 = Z t - \frac{F\left(\arcsin\left(\left(\frac{R_3 - v}{R_3 - R_2}\right)^{1/2}\right), \left(\frac{R_3 - R_2}{R_3 - R_1}\right)^{1/2}\right)}{2^{1/2}(R_3 - R_1)^{1/2}(I_{13}^2 - I_{13}I_{23} + I_{23}^2)^{1/4}}.$$
 (26)

Here F is the elliptic integral of the first kind and R_1 , R_2 , R_3 , v are explicit functions of the initial variables B_j , j = 1, 2, 3. The same is true for 2-triad clusters. With the reduction procedure [KL08], this means in particular that a resonant cluster consisting of, say, 20 or 100 modes, can theoretically be described by one dynamical invariant.

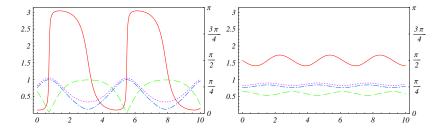
Dynamical phase. Another important fact established in our research is the effect of the dynamical phase $\varphi = \theta_1 + \theta_2 - \theta_3$ on the amplitudes a_j . It was a common belief that for an exact resonance to occur, it is necessary

¹ http://demonstrations.wolfram.com/NonlinearWaveResonances/

that φ is either zero or constant (e.g. [LHG67, Ped87]). It is evident from the Figure 13 that this is not true.

Applications

Speaking very generally, there exist two ways of using NRA for practical purposes. Kinematical methods can be used for computing the form of new technical facilities (laboratory water tank or an airplane wing or whatever else) such that nonlinear resonances will not appear. Dynamical methods should be used in case reconstruction of the laboratory facilities is too costly a game, for instance while studying stable energy states in Tokamak plasma. It costs hundreds of millions of dollars to construct a new Tokamak. On the other hand, adjustment of dynamical phases can diminish the amplitudes of resonances (in this case, these are resonantly interacting drift waves) 10 times and more for the same technical equipment as it is shown in Figure 13.



Color on-line. Plots of the modes' amplitudes and dynamical phase as functions of time, for a triad with Z=1. For each frame, the dynamical phase $\varphi(t)$ is (red) solid, $C_1(t)$ is (purple) dotted, $C_2(t)$ is (blue) dash-dotted, $C_3(t)$ is (green) dashed. Initial conditions for the amplitudes are the same for all frames; initial dynamical phase is (from the left to the right) $\varphi=0.04$ and 0.4. Here, horizontal axe denotes non-dimensional time; vertical left and right axes denote amplitude and phase correspondingly.

Figure 13

CENREC

Presently a Web portal for a virtual CEntre for Nonlinear REsonance Computations (CENREC) is being developed at RISC as an international open-source information resource in the most important and vastly developing area of modern nonlinear dynamics – nonlinear resonance analysis. CENREC will contain the following:

- 1. A MediaWiki-based hypertext encyclopedia with references to the electronic bibliography and to executable software;
- 2. An electronically indexed and searchable bibliography, with links to electronic documents (if freely available);
- 3. A collection of executable symbolic methods accessible via web interfaces (http://cenrec.risc.uni-linz.ac.at/portal/).

5.3 Highlights of the research on the NRA

$Natural\ phenomena$

Intraseasonal oscillations (IOs) in the earth's atmosphere with periods 30-100 days have been discovered in observed atmospheric data in 1960th. They play important role for modeling climate variability. All attempts to explain their origin, including numerical simulations with 120 tunable parameters, failed [GKLR04]. We developed a model of IOs based on the NRA; this model explains all known characteristics of IOs and also predict their appearance, for suitable initial conditions. The paper on the subject has been published in the journal Number 1 in general modern physics – *Physical Review Letters* (PRL, [KL07]). The model called a lot of attention of scientific community: it has been featured in "Nature Physics" (3(6): 368; 2007), listed in PRL Highlights by "The Biological Physicist" (7(2): 5; 2007), etc.

Numerics

The NRA should be regarded as a necessary preliminary step before any numerical simulations with nonlinear evolutionary dispersive PDEs. Instead of using Galerkin-type numerical methods to compute one system of 2500 interconnected nonlinear ODEs for the example regarded in Section 5.2, we have 28 small independent systems and among them 18 are *integrable analytically* in terms of special functions (e.g. in Jacobian or Weierstrass's elliptic functions, see [BK09b]). The largest system to be solved numerically consists of only 12 equations. These theoretical findings are completely general, and do not depend on the form of dispersion function and chosen spectral domain, only the form and the number of small subsystems will change (e.g. [KL08, Kar94, KK07]).

Mathematics

Nonlinear resonance analysis is a natural next step after Fourier analysis developed for linear PDEs. The necessary apparat of a new branch of math-

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ematical physics—definitions, theorems, methods, applications—is already available. The monograph on the subject, authored by E. Kartashova, will be published soon by Cambridge University Press. What is still missing, is an appropriate set of simple basis functions, similar to Fourier harmonics $\exp[i(\mathbf{k}\mathbf{x}+\omega t)]$ for linear PDEs. The form of dynamical invariants gives a hint that the functional basis of the NRA might be constructed, for instance, of three Jacobian elliptic functions \mathbf{sn} , \mathbf{dn} and \mathbf{cn} or their combinations. If this task would be accomplished, the NRA will become necessary routine part of any university education in natural sciences as is nowadays Fourier analysis.

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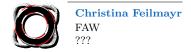


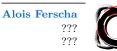
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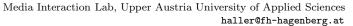






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