Computational Mathematics

Recent Developments from a Symbolic Point of View

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DK Fundamentals Lecture
January 29, 2013, JKU

Homework Problems

NOTE. The grade you obtain on this part of the "DK Fundamentals" depends on how you work out these Homework Problems.

Submit your solutions either in hardcopy or in electronic form. Deadline: basically no deadline. (But I recommed not to delay for too long;)

Homework Problem 1

Consider *Mathematica*'s output to "RSolve". Question: Is it correct?

```
re = {-F[k] - F[1 + k] + F[2 + k] == 0, F[0] == 1, F[1] == 1};
RSolve[re, F[k], k]
```

$$\left\{\left\{F[k] \to \frac{1}{2} (\text{Fibonacci}[k] + \text{LucasL}[k])\right\}\right\}$$

Homework Problem 2

Reconsider the "Automatic Proof " (given below) of the "Binomial Theorem"

$$(1) \qquad \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k} = (x+y)^n, \quad n \geq 0:$$

(a) Verify by hand the correctness of the identity (recall: $\Delta_k(f(k)) := f(k+1) - f(k)$):

$$(2) \qquad (x+y) F(n,k) - F(n+1,k) = \Delta_k (F(n,k) R(n,k))$$

where

$$F(n,k) = \binom{n}{k} x^k y^{n-k} \quad \text{and} \quad R(n,k) = \frac{k\,y}{-k+n+1}.$$

(b) Derive from (2) a valid proof of (1) by following the structure of the "Automatic Proof " derived below using the procedure call **"Prove[]**."

Homework Problem 3

Imitate the computer proof of Cassini's identity (see below) to prove the identity

$$(3) \qquad G[2n+1] = G[n]^2 + G[n+1]^2, \quad n \geq 0,$$

where G[n] is defined by the holonomic (also called: P-finite) recurrence

```
reG = {-G[n] - G[1 + n] + G[2 + n] == 0, G[0] == 0, G[1] == 1};
```

HINT : To find out how one obtains recurrences for subsequences G[a*n+b] automatically,
consult (see RISC web page) Christian Mallinger's Thesis:
"Algorithmic Manipulations and Transformations of Univariate Holonomic Functions and Sequences",
Diploma Thesis, RISC, J. Kepler University, Linz, August 1996. [pdf]

Contents of the Talk

- Computational Mathematics: A Bit of SFB History
- Computational Mathematics: A Bit of General History
- Some Symbolic Snapshots
  - Automated guessing
  - Fibonacci and automated proving

Computational Mathematics: A Bit of SFB History

The SFB “Numerical and Symbolic Scientific Computing”(1998 - 2008)
Participating institutions:

- Institute of Applied Geometry (B. Jüttler),
- Institute of Computational Mathematics (U. Langer, SFB speaker until March 2003),
- Institute for Industrial Mathematics (H. Engl),
- Research Institute for Symbolic Computation (RISC; B. Buchberger, PP, F. Winkler)
- Johann Radon Institute for Computational and Applied Mathematics (RICAM)

Overall SFB Goal

The design, verification, implementation, and analysis of numerical, symbolic, and geometrical methods for solving large-scale direct and inverse problems of high complexity. This included so-called field problems, usually described by partial differential equations (PDEs), and algebraic problems, e.g., involving constraints in algebraic formulation.

IN SHORT. Combine two different areas of computational mathematics:

NUMERICAL and SYMBOLIC COMPUTATION.
⟶ subfields of COMPUTATIONAL SCIENCE

What is COMPUTATIONAL SCIENCE?

U. Langer in his 2008 Alpach Presentation cited a definition from Wikipedia:

> ‘’COMPUTATIONAL SCIENCE is the field of study concerned with constructing
> mathematical models and numerical solution techniques
> and using computers to analyse and solve scientific, social scientific and engineerung problems.
> In practical use, it is typically the application of computer simulation and other forms of computation to problems in various scientific disciplines.’’

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JKU refinement of the Wikipedia definition!

Justification of the JKU refinement of the Wikipedia definition

From the end-evaluation (2008) of the SFB:

> “This SFB contributed significantly to the further development of basic science. They contributed to the advancement of theory (new theorems) and practice (new algorithms). These advancements have been possible by combining insights and expertise from two almost disjunct fields. An important effect of the SFB is that it had led to convergence of these fields, instead of the usual divergence and specialization that one sees so often.”

> “The SFB represents a center of excellence with very high international visibility. There is now much more serious interest from industry. Linz will become the flag place and other people would imitate it. In general, they are performing at world class level.”

SFB F013

- SFB OUTPUT:
  - 45 Master Theses, 66 Doctoral Theses, and 8 Habilitations
  - 800 articles (in refereed journals or proceedings),
  - 950 talks (at conferences/ institutions).
- SCOPE of the SFB RESULTS:
  PDE solvers, algorithms to simplify formulas/ equations, automatic proofs of mathematical statements, methods for geometric objects (curves, surfaces, etc.), regularization methods for inverse problems, symbolic/ algorithmic approaches to operator theory.
- TYPICAL APPLICATIONS:
  Problems in mechanics (structure/ thickness optimzation, flow, etc.),
  computation of electromagnetic fields, life sciences,
  engineering (FEM/ symbolics), quantum field theory (DESY),
  NIST Digital Library of Mathematical Functions (DLMF), etc..

Doctoral Program (Doktoratskolleg-DK)“Computational Mathematics”

- Start: October 1, 2008
- DK Faculty
  B. Buchberger (RISC); B. Jüttler (Geo); U. Langer (NuMa); P. Paule (DK speaker, RISC); R. Ramlau (IndMath); J. Schicho (RICAM); W. Schreiner (RISC); F. Winkler (RISC); W. Zulehner (NuMa);
  + V. Pillwein (DK Postdoc) + M. Kauers (RISC) + S. Radu (DK Postdoc)

Summary: JKU (+OeAW) Activities in Computational Mathematics

- DK (SFB) institutes: Geo, IndMath, NuMa, RISC + RICAM
- Institut für Algebra (G. Pilz);
  near-rings (structure theory + algorithms), applications of algebra, etc.
- Institut für Finanzmathematik (G. Larcher);
  quasi Monte Carlo methods, portfolio credit risk, etc.
- Institut für Wissensbasierte Mathematische Systeme (E.P. Klement);
  fuzzy logic, applied mathematics, etc.
- Institut für Stochastik (E. Buckwar);
  stochastic analysis and numerics, applications in biology, etc.
- Functional Analysis (J. Cooper);
  operators, wavelets, etc.

COMPUTATIONAL MATHEMATICS:
A Bit of General History

Pure vs. applied mathematics

G. H. Hardy (1877-1947) in his *A Mathematician's Apology* (1940):

> "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. ... Judged by all practical standards, the value of my mathematical life is nil."

Hardyism := There is something ugly about applications. - Hardy in his *Apology*:

> "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'."

With the rapid evolution of computer technology in the seventies, the position of Hardyism ***slowly*** softened up.

Gunter Dueck (who in 1987 moved to IBM from his position of a mathematics professor at the university of Bielefeld) in: *Mitteilungen der DMV 16 (2008)*:

> "Rainer Janssen (mein damaliger Manager bei IBM und heute CIO der Münchner Rück) und ich schrieben im Jahre 1991 einen Artikel mit dem Titel 'Mathematik: Esoterik oder Schlüsseltechnologie?' 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 gewählte Methode die allerbeste gewesen ist."

COMPUTATIONAL MATHEMATICS:
How is the situation today?

COMPUTATIONAL MATHEMATICS:

How is the situation today?

DIFFERENT!

COMPUTATIONAL MATHEMATICS: PURE and APPLIED

NUMERICS	and	SYMBOLICS
⊂	COMPUTATIONAL	MATHEMATICS
	⊂ **COMPUTATIONAL SCIENCE**	

Note. NUMERICS ⟷ SYMBOLICS ≈ WAVE ⟷ PARTICLE

COMPUTATIONAL MATHEMATICS:
Some Symbolic Snapshots

The following packages of my RISC Combinatorics Group are used for the following illustrative examples

```
Clear[F]
```

```
<< RISC`fastZeil`
```

Fast Zeilberger Package version 3.60
written by Peter Paule, Markus Schorn, and Axel Riese
Copyright 1995-2009, Research Institute for Symbolic Computation,
Johannes Kepler University, Linz, Austria

```
<< RISC`GeneratingFunctions`
```

Package GeneratingFunctions version 0.7 written by Christian Mallinger
Copyright 1996-2009, Research Institute for Symbolic Computation,
Johannes Kepler University, Linz, Austria

Software

- Packages of the RISC Combinatorics Group
  - Freely available at: http://www.risc.jku.at/research/combinat/software
  - More than 2,000 users world-wide. (In average two password requests per week.)
  - Audience: (pure and applied) mathematicians, but also many physicists; also engineers, etc.

InputForms: Binomials

$$\binom{n\_}{k\_}_* := \text{Binomial}[n, k]$$

$$\binom{a}{3}_*$$

$$\frac{1}{6} (-2 + a) (-1 + a) a$$

InputForms: Rising Factorials

```
(a_)k_ := Pochhammer[a, k]
```

```
{(a)0, (a)1, (a)2, (a)5}
```

{1, a, a (1 + a), a (1 + a) (2 + a) (3 + a) (4 + a)}

$$\text{FullSimplify}\left[\binom{n}{k}_{*} - \frac{(n - k + 1)_k}{(1)_k}\right]$$

0

Automatic Guessing

- **I.Q. Tests**
  Setzen Sie die Reihe fort: 1 1 2 3 5 8 13 21 ?
  Es gibt zwei Lösungsmoeglichkeiten, eine leichte und eine schwierigere. Versuchen Sie, ob Sie beide finden koennen.
  [Aufgabe 13, Denksport I für Superintelligente; ``Check Your Own I.Q.'', Hans J. Eysenck, 1966]

- **Computer Solution**
  with the RISC combinatorics package GeneratingFunctions
  [Christian Mallinger, ``Algorithmic Manipulations and Transformations of Univariate Holonomic Functions and Sequences'', Diplomarbeit, RISC-Linz, 1996]

```
GuessNext2Values[Li_] := Module[{rec}, rec = GuessRE[Li, c[k], {1, 2}, {0, 3}];
  RE2L[rec[[1]], c[k], Length[Li] + 1]]
```

```
GuessNext2Values[{1, 2, 4, 8, 16}]
```

{1, 2, 4, 8, 16, 32, 64}

```
GuessNext2Values[{1, 3, 6, 10, 15, 21}]
```

{1, 3, 6, 10, 15, 21, 28, 36}

```
GuessNext2Values[{1, 1, 2, 6, 24, 120}]
```

{1, 1, 2, 6, 24, 120, 720, 5040}

```
GuessNext2Values[{1, 1, 2, 3, 5, 8, 13, 21}]
```

{1, 1, 2, 3, 5, 8, 13, 21, 34, 55}

Book Solution

“34. (Leicht. Jede Zahl wird durch Subtraktion der folgenden von der naechstfolgenden Zahl gebildet: 2-1 = 1 usw. bis 34-21 = 13, also ist die fehlende Zahl 34.

Schwierig. Das Quadrat jeder Zahl unterscheidet sich um 1 vom Produkt der Zahlen rechts und links von ihr: $1^2 = 1$, $2 \times 1 = 2$; $2^2 = 4$, $1 \times 3 = 3$; usw. bis $21^2 = 441$, $13 \times 34 = 442$.)"

```
{1, 1, 2, 3, 5, 8, 13, 21, 34}
```

Book Solution

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{1, 1, 2, 3, 5, 8, 13, 21, 34}

Note. Die “schwierige” Lösung entspricht der Cassini (1680) Identität.

$$F[n+1]\,F[n-1] - F[n]^2 = (-1)^{n+1}, \qquad n \geq 1.$$

We shall see, this can be proved automatically with the GeneratingFunctions package!

Idea behind Automatic Guessing

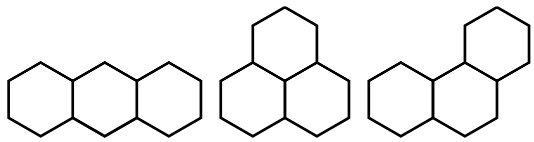
```
? GuessRE

GuessRE[{1, 2, 4, 8, 16}, c[k]]

{{-2 c[k] + c[1 + k] == 0, c[0] == 1}, ogf}

GuessRE[{1, 3, 6, 10, 15, 21}, c[k]]

{{(-3 - k) c[k] + (1 + k) c[1 + k] == 0, c[0] == 1}, ogf}

GuessRE[{1, 1, 2, 6, 24, 120}, c[k]]

{{(-1 - k) c[k] + c[1 + k] == 0, c[0] == 1}, ogf}

GuessRE[{1, 1, 2, 3, 5, 8}, F[k]]

{{-F[k] - F[1 + k] + F[2 + k] == 0, F[0] == 1, F[1] == 1}, ogf}
```

Application 1: Hexagonal Systems

Introduction (equivalence under translation, rotation and reflection)

H_n := no. of nonisomorphic hexagonal systems with n regular hexagons.

E.g.: $H_1 = 1$, $H_2 = 1$, $H_3 = 3$, $H_4 = 7$;



The Enumeration Problem

In 1999 only the values of H_1 to H_{23} were known:

```
HexSysList23 = {1, 1, 3, 7, 22, 81, 331, 1435, 6505, 30086, 141229,
   669584, 3198256, 15367577, 74207910, 359863778, 1751594643, 8553649747,
   41892642772, 205714411986, 1012565172403, 4994807695197, 24687124900540};
```

NOTE: The computation of H_{23} required 2.4 years of CPU time!

HOLONOMIC GUESSING: predicts the first 6 significant digits of H_{23} within seconds! [F. Chyzak, I. Gutman, PP, MATCH 40 (1999),139-151]

Note. For COUNTING UNDER GROUP ACTION using computer algebra see a new model for neural networks involving Hadamard patterns in: [R. Folk, A. Kartashov, P. Lisonek, and PP, “Symmetries in neural networks: a linear group action approach”, J. Phys. A: Math. Gen. 26 (1992), 3159-3164].

“Predicting H_{23}”

```
HexSysList22With5Zeros = {0, 0, 0, 0, 0, 1, 1, 3, 7, 22, 81, 331, 1435, 6505,
   30 086, 141 229, 669 584, 3 198 256, 15 367 577, 74 207 910, 359 863 778, 1 751 594 643,
   8 553 649 747, 41 892 642 772, 205 714 411 986, 1 012 565 172 403, 4 994 807 695 197};

rec = GuessRE[HexSysList22With5Zeros, a[n], {2, 2}, {7, 7}];

N[RE2L[rec[[1]], a[n], {22 + 4, 23 + 4}], 17]
```

$\{4.9948076951970000 \times 10^{12}, 2.4687137449726297 \times 10^{13}\}$

The correct value : H_{23} = 246 871 24 900 540

Predicting H_{24}, H_{25}, etc.

Other predictions are:

$$H_{24}^{*} = 122\,237\,774\,262\,384,$$
$$H_{25}^{*} = 606\,259\,305\,418\,149.$$

According to the prediction scheme the PRESUMABLE RELATIVE ERROR $\frac{H_n^{*} - H_n}{H_n}$ is 10^{-5}.

Confirmation

Predicting H_{24}, H_{25}, etc.

Other predictions are:

$$H^*_{24} = 122\,237\,774\,262\,384,$$
$$H^*_{25} = 606\,259\,305\,418\,149.$$

According to the prediction scheme the PRESUMABLE RELATIVE ERROR $\frac{H_n{}^* - H_n}{H_n}$ is 10^{-5}.

Confirmation

In [M. Vge, A.J. Guttmann, and I. Jensen, J. Chem. Inf. & Modeling 42 (2002), 456-466] the numbers H_{24} and H_{25} were computed precisely:

$$H_{24} = 122\,238\,208\,783\,203,$$
$$H_{25} = 606\,269\,126\,076\,178.$$

Application 2: Lattice Walks

Gessel's Conjecture (2001)

A *Gessel walk* in the lattice $\mathbb{Z}^2$ stays entirely in the first quadrant and consists only of the unit steps {←,→,↗,↙}.

Let G_m be the number of Gessel walks from ***(0,0)*** to ***(0,0)***.
Obviously, $G_m = 0$ if m is odd; otherwise for $m=2n$:

$$G_{2n} = 16^n \frac{(5/6)_n \, (1/2)_n}{(5/3)_n \, (2)_n} \qquad (n \geq 0).$$

Proof method (M. Kauers, C. Koutschan, and D. Zeilberger, 2008)

For G_{2n} a holonomic recurrence (of order 32, with polynomial coefficients of degree 172) is derived by *non-trivial guessing + non-trivial operator methods*.

Conclusion of [M. Kauers, C. Koutschan, and D. Zeilberger, 2008]

"(...) To that end, the third-named author (DZ) offers a prize of one hundred (100) US-dollars for a short, self-contained, human-generated (and computer-free) proof of Gessel's conjecture, not to exceed five standard pages typed in standard font.The longer that prize would remain unclaimed, the more (empirical) evidence we would have that a proof of Gessel's conjecture is indeed beyond the scope of humankind."

Fibonacci and Automatic Proving

The Fibonacci sequence (Leonardo Fibonacci, 1202)

```
GuessRE[{1, 1, 2, 3, 5, 8}, F[k]]
```

```
{{-F[k] - F[1 + k] + F[2 + k] == 0, F[0] == 1, F[1] == 1}, ogf}
```

```
re = {-F[k] - F[1 + k] + F[2 + k] == 0, F[0] == 1, F[1] == 1};
```

```
RSolve[re, F[k], k]
```

$$\left\{\left\{F[k] \to \frac{1}{2}\,(\text{Fibonacci}[k] + \text{LucasL}[k])\right\}\right\}$$

$$F[k] = \frac{1}{\sqrt{5}}\left(\left(\frac{1+\sqrt{5}}{2}\right)^{k+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{k+1}\right)$$

Fibonacci and Automatic Proving

Computer proof of Cassini identity

Recall

```
Clear[F]; re
```

```
{-F[k] - F[1 + k] + F[2 + k] == 0, F[0] == 1, F[1] == 1}
```

Proof.

```
f = DefineS[re, F[k]]
```

```
RE[{{0, -1, -1, 1}, {1, 1}}, F[k]]
```

```
Shift[f, 1] * Shift[f, -1] - f ^ 2 == DefineS[{a[n + 1] == -a[n], a[0] == -1}, a[n]]
```

RE2L::negative: Warning The recurrence is extended to (some) negative integers.

```
True
```

Fibonacci and Automatic Proving (cont.)

Fibonacci numbers as binomial sum

Recall

$$f[n\_] := \sum_{k=0}^{n} \binom{n-k}{k}_*$$

```
{f[0], f[1], f[2], f[3], f[4], f[5], f[6], f[7], f[8]}
```

```
{1, 1, 2, 3, 5, 8, 13, 21, 34}
```

These are indeed the Fibonacci numbers!

Proof.

$$\text{Unprotect[Show]; Zb}\left[\binom{n-k}{k}_*, \{k, 0, \text{Infinity}\}, n, 2\right]$$

```
{SUM[n] + SUM[1 + n] - SUM[2 + n] == 0}
```

```
Prove[]
```

An Automatic Proof of the Binomial Theorem

We prove the binomial theorem in the form

$$\sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k} = (x + y)^n$$

Set

$$g[n\_] := \sum_{k=0}^{n} \binom{n}{k}_* x^k y^{n-k}$$

```
{g[0], g[1], g[2], g[3], g[4], g[5], g[6], g[7], g[8]} // Factor
```

$\{1, x + y, (x + y)^2, (x + y)^3, (x + y)^4, (x + y)^5, (x + y)^6, (x + y)^7, (x + y)^8\}$

Proof.

Unprotect[Show]; Zb$\left[\binom{n}{k}_* x^k y^{n-k}, \{k, 0, n\}, n, 1\right]$

```
If `n' is a natural number, then:
```

$\{(x + y)\, SUM[n] - SUM[1 + n] == 0\}$

Prove[]