Symbolic Computation in Combinatorics: Recent Developments at RISC

Peter.Paule@risc.uni-linz.ac.at

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Symbolic Computation in Combinatorics

- **What does it mean?**
  - Doing heuristics with computer algebra.
  - Developing algorithms (and software) relevant to combinatorics.
  - Combining algorithms to new methods.
  - Other aspects: e.g., electronic tables for special function identitites (DLMF),databases for geometrical objects, integer sequences (N. Sloane), etc.

The RISC Castle

JSC Special Issues: Symbolic Computation in Combinatorics

- PP and D. Zeilberger (eds.), Symbolic Computation in Combinatorics, Special Issue of the J. of Symbolic Computation 14 (1992).

- PP and V. Strehl (eds.), Symbolic Computation in Combinatorics Δ_1,
Special Issue of the J. of Symbolic Computation 20

(1995). (Proceedings of the ACSyAM Workshop Sept. 21−24, 1993, Mathematical Sciences Institute, Cornell University; advising editors: G.E. Andrews, Ph. Flajolet, and D. Zeilberger.)

Some Packages of my RISC Combinatorics Group

```
SetDirectory[
 "/home/ppaule/RISC_Comb_Software
   _Sep05.dir/SumRISC"]
```

```
/home/ppaule/RISC_Comb
  _Software_Sep05.dir/SumRISC
```

```
<< SumRISC.m
```

```
Fast Zeilberger Package by Peter Paule and Markus
Schorn (enhanced by Axel Riese) – © RISC Linz – V
3.53 (02/22/05)
```

```
q-Zeilberger Package by Axel Riese – © RISC Linz –
V 2.42 (02/18/05)
```

```
Bibasic Telescope Package by Axel Riese – © RISC
Linz – V 2.24 (12/11/03)
```

```
MultiSum Package by Kurt Wegschaider (enhanced by
Axel Riese and Burkhard Zimmermann) – © RISC Linz –
V 2.02β (02/21/05)
```

```
qMultiSum Package by Axel Riese – © RISC Linz – V
2.51 (06/30/04)
```

```
GeneratingFunctions Package by Christian Mallinger
– © RISC Linz – V 0.68 (07/17/03)
```

```
SumRISC – Bundled on
  Tue Feb 22 09:37:48 CET 2005
```

Further Packages of my RISC Combinatorics Group

- **Sigma**; see e.g.: C. Schneider, "Symbolic Summation Assists Combinatorics", Sem. Lothar. Combin. 56 (2007), 1−36, B56b.
- **SumCracker**; see e.g.: M. Kauers, "A Package for Manipulating Symbolic Sums and Related Objects", Report 2005−21, SFB F013, 2005.

- **Omega**; by A. Riese (in cooperation with G.E. Andrews and PP), an implementation of an algorithmic version of MacMahon's partition analysis. See [G.E. Andrews and PP, "MacMahon's Partition Analysis XI: Broken Diamonds and Modular Forms", Acta Arithm. 126 (2007), 281−294] for further references.

Software

Freely available at:
http://www.risc.uni−linz.ac.at/research/combinat/software

Input Forms

Binomials

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

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

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

Recent Progress at RISC

Various achievements

E.g., in collaboration with colleagues from numerical analysis (FEM):

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

for $-1 \leq x \leq 1$ and $n \geq 0$. Conjectured by J. Schoeberl, proved by V. Pillwein.

Two case studies

- A Computer−Assisted Proof of Moll's Log−Concavity Conjecture
  (MultiSum + SumCracker; M. Kauers and PP; to appear: Proc. of the AMS)

- MacMahon's Dream Has Come True (Omega; G.E. Andrews and PP, "MacMahon's PA XII: Plane Partitions"; to appear: J. London Math. Soc.)

From V. Moll's Personal Story

See: Victor Moll, "The evaluation of integrals: A personal story", Notices of the AMS 49 (2002), 311−317.

NOTE: See also Moll's book (joint with George Boros): "Irresistable Integrals" [Cambride, 2004].

Starting point: Some integrals for the quartic:

$$\int_0^\infty \frac{1}{(x^4 + 6\,x^2 + 1)^1}\,dx = \frac{\pi}{4\sqrt{2}}$$

$$\int_0^\infty \frac{1}{(x^4 + 6\,x^2 + 1)^2}\,dx = \frac{9\,\pi}{64\sqrt{2}}$$

$$\int_0^\infty \frac{1}{(x^4 + 6\,x^2 + 1)^3}\,dx = \frac{219\,\pi}{2048\sqrt{2}}$$

$$\int_0^\infty \frac{1}{(x^4 + 6\,x^2 + 1)^4}\,dx = \frac{2933\,\pi}{32768\sqrt{2}}$$

Higher orders take quite a while!

$$\text{Timing}\left[\int_0^\infty \frac{1}{(x^4 + 6\,x^2 + 1)^{11}}\,dx\right]$$

$$\left\{61.56\ \text{Second},\ \frac{57143600607093\,\pi}{112589990684262 4\sqrt{2}}\right\}$$

- **Definite integrals and Mathematica**

V. Moll: "... Thus it is not entirely clear what *Mathematica* is doing to compute these integrals..."

NOTE. E.g, *MMA leaves unevaluated*

$$\int_0^\infty \frac{1}{(x^4 + 2\,a\,x^2 + 1)^{m+1}}\,dx$$

■ A double sum representation for the quartic

Theorem

Let $a > -1$ and let m be a natural number. Then

$$\int_0^\infty \frac{1}{(x^4 + 2\,a\,x^2 + 1)^{m+1}}\,dx = \frac{\pi}{2^{m+3/2}\,(a+1)^{m+1/2}} * P_m(a)$$

where

$$P_m(a) = \sum_{j,\,k} \binom{2m+1}{2j} \binom{m-j}{k} \binom{2k+2j}{k+j} \frac{(a+1)^j\,(a-1)^k}{2^{3(k+j)}}$$

PROOF

‘The proof is elementary and employs Wallis’ integral formula.’

Do we know anything about the polynomials $P_m(a)$?

■ 1 st Observation : The coefficients of $P_m(a)$ seem to be positive

$$P_m(a) = \sum_{l=0}^{m} d[l,\, m]\, a^l$$

```
d[l_, m_] :=
```

$$\sum_{j=0}^{m}\sum_{k=0}^{m-j}\sum_{i=0}^{l}\binom{2m+1}{2j} * \binom{m-j}{k} * \binom{2k+2j}{k+j} * \frac{(-1)^{k+l+i}}{2^{3(k+j)}} \binom{j}{i} * \binom{k}{l-i} *$$

```
Map[d[#, 8] &, Range[0, 8]]
```

$$\left\{\frac{4023459}{32768}, \frac{3283533}{4096}, \frac{9804465}{4096}, \frac{8625375}{2048}, \frac{9695565}{2048}, \frac{1772199}{512}, \frac{819819}{512}, \frac{109395}{256}, \frac{6435}{128}\right\}$$

POSITIVITY CONJECTURE: `d[l,m] > 0`

- **Moll et al. succeeded to derive positivity from Ramanujan's Master Theorem**

The derivation takes several non−trivial steps:

Step 1 (a consequence from the Theorem)

$$\int_0^\infty \frac{1}{b x^4 + 2 a x^2 + 1} \, dx = \frac{\pi}{2\sqrt{2}} \frac{1}{\sqrt{a + \sqrt{b}}}$$

Step 2 (V.Moll et al. connected the $P_m(a)$ to Taylor series h(c))

The Taylor series expansion of $h(x) = \sqrt{a + \sqrt{1 + x}}$,
for x in a neighborhood of the origin , is given by:

$$h(x) = \sqrt{a+1}\left(1 + \frac{1}{2}\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \frac{P_{k-1}(a)}{2^k (a+1)^k} x^k\right)$$

Step 3 (Ramanujan's Master Theorem; see e.g. B. Berndt, R's Notebooks Part I)

$$\text{If} \qquad F(x) = \sum_{k=0}^{\infty} (-1)^k \frac{f(k)}{k!} x^k$$

$$\text{then} \qquad f(-n) = \frac{1}{\Gamma(n)} \int_0^{\infty} x^{n-1} F(x)\, dx.$$

In other words,

$$\int_0^{\infty} x^{n-1} \sum_{k=0}^{\infty} (-1)^k \frac{f(k)}{k!} x^k\, dx = \Gamma(n) f(-n).$$

Define

$$B_m(a) := \int_0^{\infty} \frac{x^{m-1}}{\left(a + \sqrt{1+x}\right)^{2m+1/2}}\, dx$$

Step 4 (applying Ramanujan's Master Theorem to a suitable derivative of h(c) yields a useful integral transform)

$$B_m(a) = \frac{2^{5m}}{(a+1)^{m+1/2}} \left(m \binom{4m}{2m} \binom{2m}{2m}\right)^{-1} P_m(a)$$

Step 5 : $P_m(a)$ can be expressed as a binomial single sum

$$P_m(a) = 2^{-2m} \sum_{k=0}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} (a+1)^k$$

REMARK: (i) A concise version of Ramanujan’s Master Theorem is due to G. H. Hardy. (ii) The conditions that make the Master Theorem applicable are non−trivial to check.

SUMMARY:

$$P_m(a) = 2^{-2m} \sum_{k=0}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} (a+1)^k$$

implies POSITIVITY. Also, this SUM can be found in tables (e.g., DLMF);
it is a special instance of the Jacobi family.

BUT we shall see:

With COMPUTER ALGEBRA,
positivity and much more can be proved
in a straightforward manner !

- **Positivity derived with MULTISUM [M. Kauers & PP, 2006]**

Recall that

$$P_m(a) = \sum_{l=0}^{m} d[l, m]\, a^l$$

where

$$d[l\_,\ m\_] := \sum_{j=0}^{m} \sum_{k=0}^{m-j} \sum_{i=0}^{l} \binom{2m+1}{2j}_* \binom{m-j}{k}_* \binom{2k+2j}{k+j}_* * \frac{(-1)^{k+l+i}}{2^{3(k+j)}} \binom{j}{i}_* \binom{k}{l-i}_*$$

$$\text{summand} = \binom{2m+1}{2j}_* \binom{m-j}{k}_* \binom{2k+2j}{k+j}_* \frac{(-1)^{k+l+i}}{2^{3(k+j)}} * \binom{j}{i}_* * \binom{k}{l-i}_* ;$$

```
SetOfShifts =
 FindStructureSet[summand, {l, m},
  {1, 0}, {k, j, i}, {0, 1, 0}, 1];
StructSet = SetOfShifts[[2]];
```

```
FindRecurrence[summand, {l, m},
 {k, j, i}, StructSet, 1, WZ → True]
```

$$\{-4\,(l+m)\,F[-1+l,\,m,\,-1+k,\,-1+j,\,-1+i]-2\,(3+2\,l+4\,m)\,F[l,\,m,\,-1+k,\,-1+j,\,-1+i]+4\,(1+m)\,F[l,\,1+m,\,-1+k,\,-1+j,\,-1+i]==$$
$$\Delta_i[(-7+6\,j+2\,k)\,F[-1+l,\,m,\,-1+k,\,-1+j,\,-1+i]+2\,(3+2\,l+4\,m)\,F[l,\,m,\,-1+k,\,-1+j,\,-1+i]-4\,(1+m)\,F[l,\,1+m,\,-1+k,\,-1+j,\,-1+i]]+$$
$$\Delta_j[(-7+6\,j+2\,k)\,F[-1+l,\,m,\,-1+k,\,-1+j,\,i]+(-1+2\,j+2\,k+4\,m)\,F[l,\,m,\,-1+k,\,-1+j,\,i]-4\,(1+m)\,F[l,\,1+m,\,-1+k,\,-1+j,\,i]]+$$
$$\Delta_k[(7-6\,j-2\,k+4\,l+4\,m)\,F[-1+l,\,m,\,-1+k,\,-1+j,\,-1+i]-4\,(j+k-l)\,F[-1+l,\,m,\,k,\,-1+j,\,-1+i]+(7-2\,j-2\,k+4\,l+4\,m)\,F[l,\,m,\,-1+k,\,-1+j,\,i]+4\,(2\,j+k+m)\,F[l,\,m,\,-1+k,\,j,\,i]-4\,(k-l)\,F[l,\,m,\,k,\,-1+j,\,i]-4\,(1+m)\,F[l,\,1+m,\,-1+k,\,j,\,i]]\}$$

```
SumCertificate[%]
```

$$\{-2\,(l+m)\,SUM[-1+l,\,m]+(-3-2\,l-4\,m)\,SUM[l,\,m]+2\,(1+m)\,SUM[l,\,1+m]==0\}$$

In other words, the RISC package MULTISUM found that for ***0≤l≤m+1***:

$$d[l,\,m+1]=\frac{4\,m+2\,l+3}{2\,(m+1)}\,d[l,\,m]+\frac{m+l}{m+1}\,d[l-1,\,m]$$

This recurrence implies POSITIVITY of all the ***d[l,m]***! (NOTE: ***d[0,0]*** =1.)

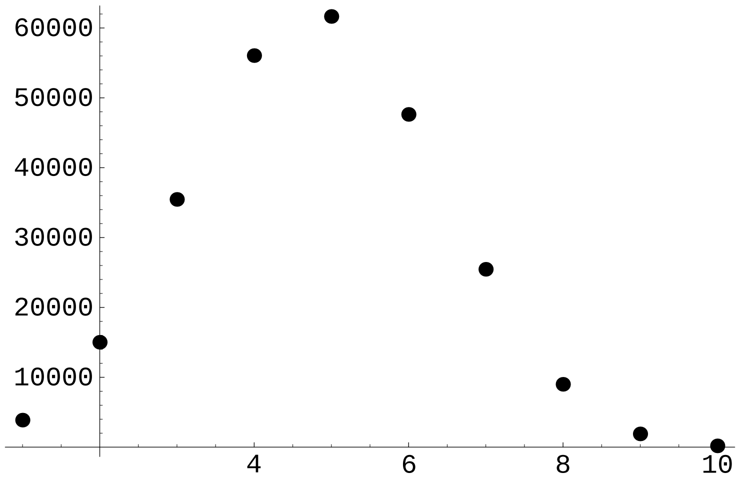
Moll's Log–Concavity Conjecture

■ 2 nd Observation :

The coefficients of $P_m(a)$ seem to be unimodal

```
Coeffs = Map[N[d[#, 10]] &, Range[10]];

ListPlot[Coeffs,
 PlotStyle → PointSize[0.02]];
```

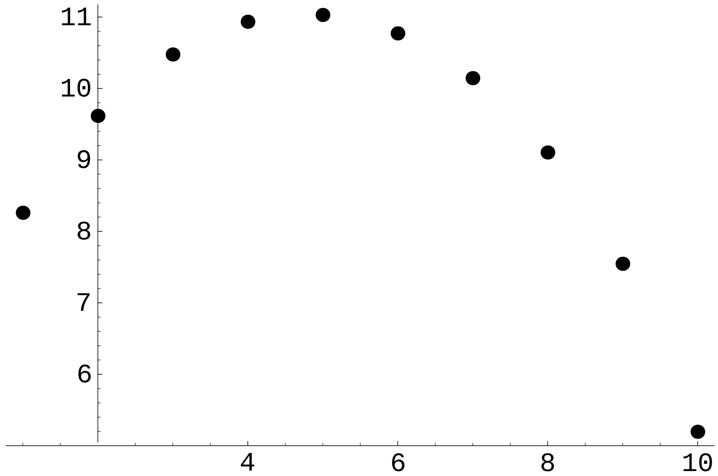


NOTE. Boros & Moll (1999) proved unimodality of the ***d[l,m]*** based on the Jabobi single sum representation of $P_m(a)$.

■ 3 rd Observation :

The coefficients of $P_m(a)$ seem to be also log − concave

```
ListPlot[N[Log[Coeffs]],
 PlotStyle → PointSize[0.02]];
```



CONCAVITY: For $D[l,m] := Log(d[l,m])$,

$$\frac{D[l-1,m] + D[l+1,m]}{2} \leq D[l,m]$$

CONCAVITY: For $D[l,m] := Log(d[l,m])$,

$$\frac{D[l-1,m] + D[l+1,m]}{2} \leq D[l,m]$$

Recall : $P_m(a) = \sum_{l=0}^{m} d[l,m]\, a^l$

LOG−CONCAVITY CONJECTURE: *For $0 < l < m$,*

$$d[l-1,m]\, d[l+1,m] \leq d[l,m]^2$$

NOTE 1:

LOG−CONCAVITY ⟹ UNIMODALITY

NOTE 2. The conjecture was raised by Victor Moll (~ 1998); all know classical approaches failed.

The Proof

We need the following ingredients:
(0) positivity d[l,m]>0;
(1) Collins' Cylindrical Algebraic Decomposition (CAD);
(2) Kauers' package SumCracker applied to inequalities − based on an algorithm by Gerhold/Kauers (ISSAC'05);
(3) recurrences delivered by Wegschaider's package MultiSum; namely,

$$Rec_1 = Rec_1\,(d[l-1, m], d[l, m], d[l, m+1])$$

(the positivity recurrence from above),

$$Rec_2 = Rec_2\,(d[l, m], d[l, m+1], d[l+1, m]),$$

NOTE. $d[l-1, m]\, d[l+1, m] \le d[l, m]^2$

$$Rec_3 = Rec_3\,(d[l, m], d[l, m+1], d[l, m+2])$$

Invoking Rec_1 and Rec_2 one obtains: For $0 < l < m$ the

LOG – CONCAVITY CONJECTURE

is equivalent to

$$q_1 * d[l, m]^2 + q_2 * d[l, m] + q_3 * d[l, m+1]^2 \le 0,$$

where the $q_i = q_i[l, m]$ are polynomials in l and m.

Invoking CAD one obtains: If $0 < l < m$, then

$$q_1 * d[l, m]^2 + q_2 * d[l, m] + q_3 * d[l, m+1]^2 \leq 0,$$

is violated at points (l, m) if and only if

$$\frac{p_1 - \sqrt{p_2}}{p_3} * d[l, m] < d[l, m+1] < \frac{p_1 + \sqrt{p_2}}{p_3} * d[l, m]$$

where the $p_i = p_i[l, m]$ are polynomials in l and m.

HENCE TO COMPLETE THE PROOF IT SUFFICES TO SHOW THAT

$$d[l, m+1] \geq \frac{p_1 + \sqrt{p_2}}{p_3} * d[l, m]$$

FOR $0 < l < m$.

FURTHER PROBLEM SIMPLIFICATION:
Suppose
$u = u[l, m]$ is a poly in l and m such that $u[l, m] \geq 0$ for $0 < l < m$, then to show

$$d[l, m+1] \geq \frac{p_1 + \sqrt{p_2}}{p_3} * d[l, m],$$

it suffices to show

$$d[l, m+1] \geq \frac{p_1 + \sqrt{p_2 + u}}{p_3} * d[l, m]$$

CHOOSING $u := l^2 (2 l + 1)^2 - p_2$

turns the last inequality into the following condition:

$$d[l, m+1] \geq \frac{4m^2 + 7m + l + 3}{2(m+1-l)(m+1)} * d[l, m].$$

SUMMARIZING: The log−concavity conjecture is equivalent to

$$d[l, m+1] \geq \frac{4m^2 + 7m + l + 3}{2(m+1-l)(m+1)} * d[l, m] \quad (0 < l < m).$$

This can be proved automatically by Kauers' SumCracker package.

NOTE: As additional input, Rec_3 (being with respect to m only) is given to serve as the defining relation for the $d[l,m]$. Q.E.D.

MacMahon's Partition Analysis and the Omega Package

■ Loading the Omega Package

```
SetDirectory[
 "/home/ppaule/RISC_Comb_Software
   _Sep05.dir/Omega/"]
```

```
/home/ppaule/RISC_Comb
  _Software_Sep05.dir/Omega
```

```
<< Omega2.m
```

```
Omega Package by Axel Riese (in cooperation with
George E. Andrews and Peter Paule) — © RISC Linz —
V 2.47 (06/21/05)
```

■ Triangles with sides of integer length

PROBLEM* (e.g., R.Stanley,1986): Let *t(n)* be the number of non-congruent triangles with sides of integer length and with perimeter n. *Find

$$T(q) := \sum_{n=3}^{\infty} t(n)\, q^n$$

Example: $t(9) = 3$ corresponding to 1+4+4, 2+3+4, 3+3+3,

$$T(q) = \sum_{\substack{a,b,c\geq 1 \\ a\leq b\leq c,\ a+b>c}} q^{a+b+c} = ?$$

$$T(q) = \sum_{\substack{a,b,c\geq 1 \\ a\leq b\leq c,\ a+b>c}} q^{a+b+c} =$$

$$= \underset{\geq}{\Omega} \sum_{a,b,c\geq 1} \lambda_1^{b-a} \lambda_2^{c-b} \lambda_3^{a+b-c-1} q^{a+b+c}$$

$$= \underset{\geq}{\Omega} \frac{q^3}{\left(1-\frac{q\lambda_2}{\lambda_3}\right)\left(1-\frac{q\lambda_3}{\lambda_1}\right)\left(1-\frac{q\lambda_1\lambda_3}{\lambda_2}\right)}$$

In such situations MacMahon eliminated the λ
by applying successively basic elimination rules such as

$$\underset{\geq}{\Omega} \frac{1}{(1-x\lambda)\left(1-\frac{y}{\lambda}\right)} = \frac{1}{(1-x)(1-xy)}.$$

REMARK: MacMahon's Omega Operator $\underset{\geq}{\Omega}$:

$$\underset{\geq}{\Omega} \sum_{s_1=-\infty}^{\infty} \cdots \sum_{s_r=-\infty}^{\infty} A_{s_1,\ldots,s_r} \lambda_1^{s_1} \cdots \lambda_r^{s_r} := \sum_{s_1=0}^{\infty} \cdots \sum_{s_r=0}^{\infty} A_{s_1,\ldots,s_r}.$$

Recall:

$$\underset{\geq}{\Omega} \frac{1}{(1 - x\lambda)\left(1 - \frac{y}{\lambda}\right)} = \frac{1}{(1-x)(1-xy)}.$$

This way one finds that

$$T(q) = \underset{\geq}{\Omega} \frac{q^3}{\left(1 - \frac{q\lambda_2}{\lambda_3}\right)\left(1 - \frac{q\lambda_3}{\lambda_1}\right)\left(1 - \frac{q\lambda_1\lambda_3}{\lambda_2}\right)}$$

$$= \underset{\geq}{\Omega} \frac{q^3}{\left(1 - \frac{q}{\lambda_3}\right)\left(1 - \frac{q\lambda_3}{\lambda_1}\right)(1 - q^2\lambda_1)}$$

$$= \underset{\geq}{\Omega} \frac{q^3}{\left(1 - \frac{q}{\lambda_3}\right)(1 - q^3\lambda_3)(1 - q^2)}$$

$$= \frac{q^3}{(1-q^4)(1-q^3)(1-q^2)}$$

With the package Omega all steps are carried out automatically:

```
OSum[q^(a+b+c), {1 ≤ a, 1 ≤ b, 1 ≤ c, a ≤ b,
   b ≤ c, a + b > c}, λ]
```

$$\underset{\substack{\geq \\ \lambda_1,\lambda_2,\lambda_3}}{\Omega} \frac{q^3}{\left(1 - \frac{q\lambda_2}{\lambda_3}\right)\left(1 - \frac{q\lambda_3}{\lambda_1}\right)\left(1 - \frac{q\lambda_1\lambda_3}{\lambda_2}\right)}$$

OR[%]

```
Eliminating λ2...
Eliminating λ3...
Eliminating λ1...
```

$$\frac{q^3}{(1-q^2)(1-q^3)(1-q^4)}$$

REMARKS

- Omega (resp. Partition Analysis) has been used extensively for mathematical discovery; e.g., k−gons, partition diamonds, magic squares, etc.

- Extensions, related combinatorial studies, Maple software:
  S. Corteel, G. Han, C. Savage, G. Xin, and others.

- Alternative approaches with similar goals:
  J. Stembridge's posets package; based on R. Stanley's work ("Ordered Structures and Partitions", Memoirs AMS 119, 1972);
  LattE (J.A. DeLoera, R. Hemmecke, R. Tanzer, R. Yoshida), an implementation of work of A. Barvinok and J. Pommersheim ("An algorithmic theory of lattice points in polyhedra", MSRI Publ. 38, 1999).