# Let's talk about Software

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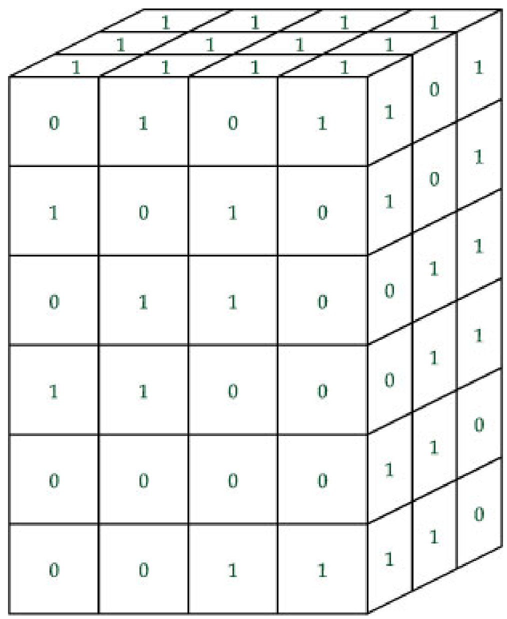
# One Problem

# Sampling/moves on 3-way tables – Markov bases



Markov basis $\subseteq$ Gröbner basis $\subseteq$ Graver basis

# One Answer

# $4_{\mathsf{ti}}2$

by R. & R. Hemmecke

downloadable from www.4ti2.de

# $4_{\mathbf{ti}}2$

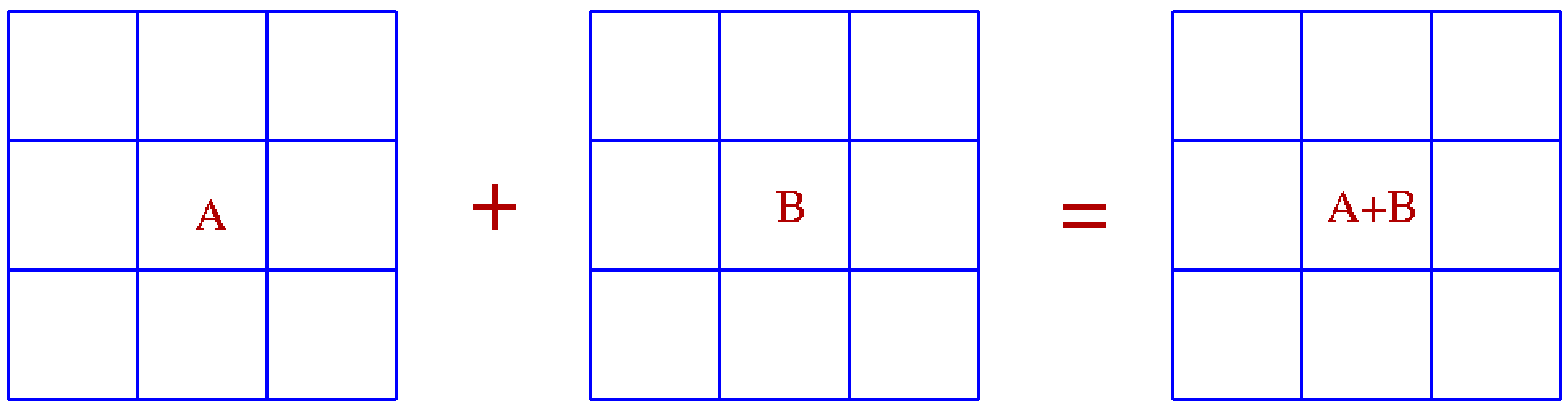
- (truncated) Hilbert bases
  - $6 \times 6$ magic squares ($\sim 500,000$ elements, $\sim 10$ days)
- (truncated, symmetric) Graver bases
  - hppi's of order $20$ ($\sim 1,250,000$ elements, $\sim 1$ month)
- (symmetric) Gröbner bases for graded toric ideals
  - $3 \times 4 \times 5$ tables ($\sim 77,000$ elements, $\sim 4$ days)
  - binary $K_5$ model ($\sim 13,000$ elements, $\sim 30$ hours)

# Challenges for $4_{\text{ti}}2$

- redo $4 \times 4 \times 4$ tables (Sawae et al.)
- Sullivant: verify that a given set of $145,512$ binomials generate the toric ideal for $4 \times 4 \times 4$ tables
- Hosten: binary $K_6$ model and its submodels
- Sturmfels: binary octahedron model
- $3 \times 3 \times 3 \times 3$ tables

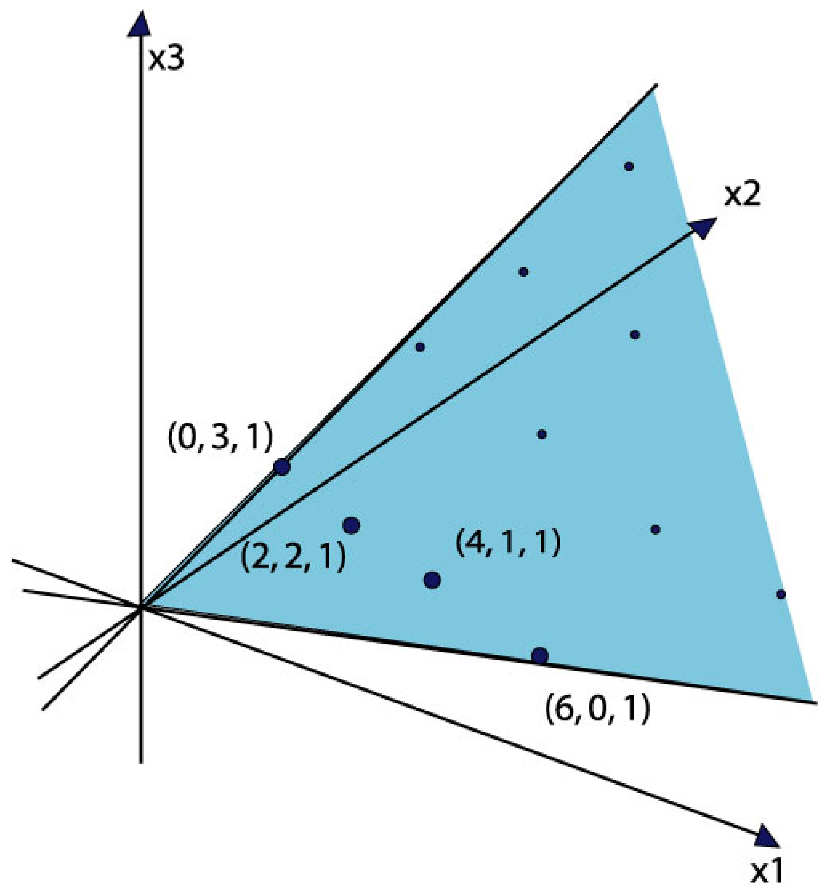
# Let's do some magic with $4_{\text{ti}}2$

# Hilbert bases and magic squares




Lemma: The set of non-negative real magic squares forms a cone.

# What is a Hilbert basis?




$$(0,3,1) \quad (2,2,1) \quad (4,1,1) \quad (6,0,1)$$

# Solving the problem with $4_{\text{ti}}2$

Consider the pointed rational cone of magic squares:

$$\ker(A) \cap \mathbb{R}^n_+ = \{z : Az = 0, z \in \mathbb{R}^n_+\}.$$

Every row, column and diagonal sum equals the sum of the first row.

# Input file: 3x3magic

```
9 7
1 1 1 -1 -1 -1  0  0  0
1 1 1  0  0  0 -1 -1 -1
0 1 1 -1  0  0 -1  0  0
1 0 1  0 -1  0  0 -1  0
1 1 0  0  0 -1  0  0 -1
0 1 1  0 -1  0  0  0 -1
1 1 0  0 -1  0 -1  0  0
```

# Call $4_{\mathbf{ti}}2$

```
./hilbert 3x3magic
```

# Output file: 3x3magic.hil

```
9 5
1 2 0 0 1 2 2 0 1
0 2 1 2 1 0 1 0 2
1 1 1 1 1 1 1 1 1
2 0 1 0 1 2 1 2 0
1 0 2 2 1 0 0 2 1
```

# Hilbert basis: $3 \times 3$ magic squares

| | | |
|---|---|---|
| 1 | 0 | 2 |
| 2 | 1 | 0 |
| 0 | 2 | 1 |

| | | |
|---|---|---|
| 2 | 0 | 1 |
| 0 | 1 | 2 |
| 1 | 2 | 0 |

| | | |
|---|---|---|
| 0 | 2 | 1 |
| 2 | 1 | 0 |
| 1 | 0 | 2 |

| | | |
|---|---|---|
| 1 | 2 | 0 |
| 0 | 1 | 2 |
| 2 | 0 | 1 |

| | | |
|---|---|---|
| 1 | 1 | 1 |
| 1 | 1 | 1 |
| 1 | 1 | 1 |

# Generating Function of $3 \times 3$ Magic Squares

Generating function of $3 \times 3$ magic squares

$$g_3(t) = \frac{(t^3+1)^2}{(1-t^3)^3} = \sum \left( \begin{array}{c} \#3 \times 3 \\ \text{magic squares} \\ \text{with sum } s \end{array} \right) t^s$$

The number of $3 \times 3$ magic squares of sum $s$ is

$$M_3(s) = \begin{cases} \frac{2}{9}s^2 + \frac{2}{3}s + 1 & \text{if } 3|s, \\ 0 & \text{otherwise,} \end{cases}$$

This final series computation was done by CoCoA.

# New Formulas for Magic and Semi-Magic Cubes

**Theorem** [Ahmed, De Loera, H.] The number of $3 \times 3 \times 3$ "semi-magic" cubes is

$$\begin{cases} \frac{9}{2240}\,s^8 + \frac{27}{560}\,s^7 + \frac{87}{320}\,s^6 + \frac{297}{320}\,s^5 + \frac{1341}{640}\,s^4 + \frac{513}{160}\,s^3 + \frac{3653}{1120}\,s^2 + \frac{627}{280}\,s + 1 & \text{if } 2|s, \\ \frac{9}{2240}\,s^8 + \frac{27}{560}\,s^7 + \frac{87}{320}\,s^6 + \frac{297}{320}\,s^5 + \frac{1341}{640}\,s^4 + \frac{513}{160}\,s^3 + \frac{3653}{1120}\,s^2 + \frac{4071}{2240}\,s + \frac{47}{128} & \text{otherwise.} \end{cases}$$

**Theorem**[Ahmed, De Loera, H.] The number of $3 \times 3 \times 3$ magic cubes is

$$MC_3(s) = \begin{cases} \frac{11}{324}s^4 + \frac{11}{54}s^3 + \frac{25}{36}s^2 + \frac{7}{6}s + 1 & \text{if } 3|s, \\ 0 & \text{otherwise.} \end{cases}$$

Computations were done by $4_{\text{ti}}2$ and CoCoA.

# What is a Graver basis?

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$$G(A) = \bigcup_j H(\ker(A) \cap \mathbb{O}_j)$$

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Fact: The Graver basis of $A$ contains the Markov basis of $A$.

# $3 \times 3$ tables

```
9 6
1 1 1 0 0 0 0 0 0
0 0 0 1 1 1 0 0 0
0 0 0 0 0 0 1 1 1
1 0 0 1 0 0 1 0 0
0 1 0 0 1 0 0 1 0
0 0 1 0 0 1 0 0 1
```

# Call $4_{\mathbf{ti}}2$

```
./graver 3x3
```

or

```
./groebner 3x3
```

# Output file: 3x3.gra

```
9 15
-1  1  0  1 -1  0  0  0  0
 0  0  0  1  0 -1 -1  0  1
-1  0  1  1  0 -1  0  0  0
 1 -1  0  0  0  0 -1  1  0
 0  0  0  1 -1  0 -1  1  0
-1  1  0  1  0 -1  0 -1  1
 0 -1  1  1  0 -1 -1  1  0
 1 -1  0  0  1 -1 -1  0  1
-1  0  1  0  0  0  1  0 -1
...
```

# Let us exploit symmetry

# Define symmetry group: 3x3.sym

```
9 4
2 3 1 5 6 4 8 9 7
2 1 3 5 4 6 8 7 9
4 5 6 7 8 9 1 2 3
4 5 6 1 2 3 7 8 9
```

# Call $4_{\mathbf{ti}}2$ with symmetry

```
./graver symmetry 3x3
```

or just

```
./graver sym 3x3
```

which creates a file 3x3.sgra

# Call $4_{\mathsf{ti}}2$ with symmetry

```
./graver symmetry 3x3
```

or just

```
./graver sym 3x3
```

which creates a file 3x3.sgra and then type

```
./output 3way 3 3 1 3x3.sgra
```

which creates a file 3x3.sgra.3way

# Output file: 3x3.sgra.3way

```
3 3 1
===============
 0  0  0
 1  0 -1
-1  0  1
===============
 0  1 -1
 1 -1  0
-1  0  1
===============
```

# Two representatives up to symmetry

$$\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{pmatrix}$$

# $3 \times 3 \times 4$ **tables**

| | Gröbner | symmGröbner | Graver | symmGraver |
|---|---|---|---|---|
| Elements | 626 | 9 | 19,722 | 37 |
| Time | 47 | 447 | 1978 | 437 |

# Another Problem

# Is there a table?

| | | | | |
|---|---|---|---|---|
| ? | ? | ? | ? | 220 |
| ? | ? | ? | ? | 215 |
| ? | ? | ? | ? | 93 |
| ? | ? | ? | ? | 64 |
| 108 | 286 | 71 | 127 | |

There is an integer solution to $Ax = b, x \geq 0$ if and only if there is a minimal solution to $(A| - b)y = 0, y \geq 0$ with last component $1$.

# Is there a table?

| | | | | |
|---|---|---|---|---|
| ? | ? | ? | ? | 220 |
| ? | ? | ? | ? | 215 |
| ? | ? | ? | ? | 93 |
| ? | ? | ? | ? | 64 |
| 108 | 286 | 71 | 127 | |

There is an integer solution to $Ax = b, x \geq 0$ if and only if there is a minimal solution to $(A| - b)y = 0, y \geq 0$ with last component $1$.

In this way, you may find that Hosten's $2 \times 3 \times 3$ table has only $441$ solutions.

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# How many tables are there?

| | | | | |
|---|---|---|---|---|
| 68 | 119 | 26 | 7 | 220 |
| 20 | 84 | 17 | 94 | 215 |
| 15 | 54 | 14 | 10 | 93 |
| 5 | 29 | 14 | 16 | 64 |
| 108 | 286 | 71 | 127 | |

# How many tables are there?

| | | | | |
|---|---|---|---|---|
| 68 | 119 | 26 | 7 | 220 |
| 20 | 84 | 17 | 94 | 215 |
| 15 | 54 | 14 | 10 | 93 |
| 5 | 29 | 14 | 16 | 64 |
| 108 | 286 | 71 | 127 | |

There are 1,225,914,276,768,514 such tables.

# How many tables are there???

| | | | | | |
|---|---|---|---|---|---|
| ? | ? | ? | ? | ? | 338106 |
| ? | ? | ? | ? | ? | 574203 |
| ? | ? | ? | ? | ? | 678876 |
| ? | ? | ? | ? | ? | 1213008 |
| 20202 | 142746 | 410755 | 1007773 | 1222717 | |

# Another Answer

# LattE - Counting lattice points

- software package developed at UC Davis (De Loera, H., Tauzer, Yoshida)
- computes number of lattice points in any rational polytope

$$Ax = a, Bx \geq b$$

- includes several algorithms to count lattice points

www.math.ucdavis.edu/∼latte

# One way to count

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Define generating function

$$g_P(z) = \sum_{\alpha \in P} z^{\alpha}$$

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Define generating function

$$g_P(z) = \sum_{\alpha \in P} z^\alpha$$

Then the number of lattice points is

$$g_P(\mathbf{1}) = \sum_{\alpha \in P} 1$$

# Life is not always easy

# A closer look onto this approach

Problem: $g_P(z)$ written as a polynomial is far too big.

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Solution: Write $g_P(z)$ as a sum of rational functions $p(z)/q(z)$.

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Solution: Write $g_P(z)$ as a sum of rational functions $p(z)/q(z)$.

Barvinok: There is always a short (polynomial size) representation of $g_P(z)$.

# Problems solved

- recomputation of counts from literature

- recomputation of counting formulas for $3 \times 3 \times 3$ magic and semi-magic cubes

- Aardal's Frobenius problems

- $3 \times 3 \times 4$ tables for given marginals

- some new counting formulas ($24$-cell, . . . )

# Challenges for LattE

- new counting formulas for $4 \times 4 \times 4$ magic and semi-magic cubes
- new counting formula for $5 \times 5$ magic squares
- your problems?!

$4_{\mathrm{ti}}2$

www.4ti2.de

# LattE

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