Sphere Packing with SDP

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Based on joint work with Rudi Pendavingh

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A drama in four acts

I. Sphere packing
II. Lattices and quadratic forms
III. Semidefinite programming and branch and bound
IV. Future work
Part I
Sphere Packing
Sphere Packing Problem

**Sphere packing:** arrangement of equal, nonoverlapping spheres in $\mathbb{R}^n$.

**Density:** Fraction of space covered by spheres.

**Problem:** Find the densest packing of spheres.
Kepler’s Conjecture, Hales’ Theorem

Theorem (Fejes Tóth, 1940).
The densest packing of circles in the plane is the hexagonal packing.

Conjecture (Kepler).
The densest packing of spheres in $\mathbb{R}^3$ is the face-centered cubic packing.
Kepler’s Conjecture, Hales’ Theorem

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Theorem (Hales, 2003).
The densest packing of spheres in $\mathbb{R}^3$ is the face-centered cubic packing.
(99% certain. Gigabytes of data plus 100 pages. Computer-verified proof underway)
Lower and upper bounds
See Figure 1 of (Cohn and Elkies, 2003)
Periodic packings

- Full-dimensional set of translations
- Fundamental *parallelotope*:
Periodic packings

- Full-dimensional set of translations
- Fundamental *parallelotope*:
Periodic packings

• *Just as hard:* truncate arbitrary packing and repeat

Lattice packings

**Definition.**

*Lattice:* discrete subgroup of $\mathbb{R}^n$.

$L = \{Bx : x \in \mathbb{Z}^n\}$ with columns of $B$ independent

*Spheres centered on lattice points*
Lattice packings

- Best lattice packing known for $n \leq 8$ and $n = 24$
- $n \leq 4$: Korkin and Zolotarev 1873
- $n = 5$: Korkin and Zolotarev 1877
- $n \leq 8$: Blichfeldt 1935
- $n = 24$: Cohn and Kumar 2003
**Lattice packings**

- Best lattice packing known for $n \leq 8$ and $n = 24$
- For $n \leq 5$: analogs of face-centered cubic, $D_n$
- For $n = 8$: fit together two $D_8$s to get $E_8$
- $E_6, E_7$ from $E_8$
- $\Lambda_{24}$ is the *Leech Lattice*

**Bounds**

- For $24 \neq n > 8$, nothing known beyond general packing bounds
- For $n = 10, 11, 13$ known non-lattice packing denser than best *known* lattice
Part II
Lattices and Quadratic Forms
Lattice packing

- Spheres centered on lattice points
- Fundamental Parallelotope has *one* sphere
- Max radius of sphere: *minimum distance*
• $L = \{Bx : x \in \mathbb{Z}^n\}$
• Volume of parallelotope: $\text{Volume}(L) = |\det(B)|$
• $d_L$ length shortest vector of $L$
• $V_n$ volume of radius-1 sphere

\[
\text{Density} = \frac{V_n(d_L/2)^n}{\text{Volume}(L)} = V_n/2^n \left( \frac{d_L^2}{\text{Volume}(L)^{2/n}} \right)^{n/2}
\]
\begin{itemize}
\item \( L = \{ Bx : x \in \mathbb{Z}^n \} \)
\item Volume of parallelotope: \( \text{Volume}(L) = |\text{det}(B)| \)
\item \( d_L \) length shortest vector of \( L \)
\item \( V_n \) volume of radius-1 sphere
\item \[
\gamma_n = \max \left\{ \frac{d_L^2}{\text{Volume}(L)^{2/n}} : L \text{ is } n - \text{dim. lattice} \right\}
\end{itemize}
Aside: Basis Reduction

- Given $L$, find shortest vector: **NP-hard**
- Approximation algorithm: LLL. Factor $2^{n/2}$. Applications:
  - Factoring polynomials
  - Integer Programming in fixed dimension
  - Hidden structure in integer programs (Market Split Problem)
  - Crypto
  - Find exact shortest vector in fixed dimension
  - . . .
Korkin-Zolotarev Reduction
Korkin-Zolotarev Reduction
Korkin-Zolotarev Reduction
Korkin-Zolotarev Reduction
Positive Definite Quadratic forms

Definition.
A quadratic form \( q(x_1, \ldots, x_n) = \sum_{i,j} q_{ij} x_i x_j \) is positive definite if

- \( q(x) \geq 0 \) for all \( x \in \mathbb{R}^n \)
- \( q(x) = 0 \) iff \( x = 0 \)

The minimum is \( m(q) := \min \{ q(x) : x \in \mathbb{Z}^n, x \neq 0 \} \)
Hermite’s Constant

- \( L = \{ Bx : x \in \mathbb{Z}^n \} \)
- Volume of parallelotope: \( \text{Volume}(L) = |\det(B)| \)
- \( \gamma_n = \max \left\{ \frac{d_L^2}{\text{Volume}(L)^{2/n}} : L \text{ is } n - \text{dim. lattice} \right\} \)

Quadratic form: \( q(x) = x^TQx = x^TB^TBx \)

- \( m(q) = d_L^2 \)
- \( \det(Q) = \text{Volume}(L)^2 \)
Hermite’s Constant

- $L = \{ Bx : x \in \mathbb{Z}^n \}$
- Volume of parallelotope: $\text{Volume}(L) = |\det(B)|$
- $\gamma_n = \max \left\{ \frac{m(q)}{\det(Q)^{1/n}} : q \text{ is } n\text{-var. PD quadr. form} \right\}$

Quadratic form: $q(x) = x^TQx = x^TB^TBx$

- $m(q) = d_L^2$
- $\det(Q) = \text{Volume}(L)^2$
Korkin-Zolotarev Reduction

Definition.
Lagrange expansion of $q(x)$:

$$q(x_1, x_2, x_3) = A_1(x_1 - \alpha_{12}x_2 - \alpha_{13}x_3)^2 + A_2(x_2 - \alpha_{23}x_3)^2 + A_3x_3^2$$
Korkin-Zolotarev Reduction

\[ q(x) = \sum_{i=1}^{n} A_i(x_i - \sum \alpha_{ij} x_j)^2 \] is KZ-reduced if

- \( A_1 = m(q) \)
- \( \sum_{i=2}^{n} A_i(x_i - \sum \alpha_{ij} x_j)^2 \) is KZ-reduced
- \( 0 \leq \alpha_{12} \leq 1/2 \)
- \( -1/2 \leq \alpha_{1j} \leq 1/2 \) for \( j = 3, \ldots, n \)
Hermite’s Constant

\[
\gamma_n = \max \left\{ \frac{m(q)}{\det(Q)^{1/n}} : q \text{ is } n\text{-var. PD quadr. form} \right\}
\]

\[
= \max \left\{ \frac{A_1}{(A_1A_2\cdots A_n)^{1/n}} : A_i \text{ from KZ-reduced form} \right\}
\]
First KZ-inequality

- $A_1 = m(q)$
- $\sum_{i=2}^{n} A_i(x_i - \sum \alpha_{ij}x_j)^2$ is KZ-reduced
- $0 \leq \alpha_{12} \leq 1/2$
- $-1/2 \leq \alpha_{1j} \leq 1/2$ for $j = 3, \ldots, n$

Theorem (Korkin and Zolotarev, 1873).

$$A_2 \geq \frac{3}{4}A_1$$
Second KZ-inequality

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Theorem (Korkin and Zolotarev, 1873).

\[ A_2 \geq \frac{3}{4} A_1 \]
\[ A_3 \geq \frac{2}{3} A_1 \]
Second KZ-inequality

- \( A_1 = m(q) \)
- \( \sum_{i=2}^{n} A_i(x_i - \sum \alpha_{ij}x_j)^2 \) is KZ-reduced
- \( 0 \leq \alpha_{12} \leq \frac{1}{2} \)
- \( -\frac{1}{2} \leq \alpha_{1j} \leq \frac{1}{2} \) for \( j = 3, \ldots, n \)

Theorem (Korkin and Zolotarev, 1873).

\[
A_2 \geq \frac{3}{4}A_1 \\
A_3 \geq \frac{2}{3}A_1 \\
A_4 \geq \frac{1}{2}A_1
\]
**New KZ-inequalities**

- \( A_1 = m(q) \)
- \( \sum_{i=2}^{n} A_i(x_i - \sum \alpha_{ij}x_j)^2 \) is KZ-reduced
- \( 0 \leq \alpha_{12} \leq 1/2 \)
- \( -1/2 \leq \alpha_{1j} \leq 1/2 \) for \( j = 3, \ldots, n \)

**Theorem (Pendavingh and vZ, 2007).**

\[
A_5 \geq \left( \frac{15}{32} - 10^{-5} \right) A_1 \quad (1)
\]
\[
-5A_1 + 2A_4 + 8A_5 \geq -3 \cdot 10^{-4} A_5 \quad (2)
\]
\[
-4A_1 - 3A_3 + 4A_4 + 8A_5 \geq -5 \cdot 10^{-5} A_5 \quad (3)
\]
Hermite’s constant

\[
\gamma_n = \max \left\{ \frac{A_1}{(A_1 A_2 \cdots A_n)^{1/n}} : A_i \text{ from KZ-reduced form} \right\}
\]

\[
\leq \max \left\{ \frac{A_1}{(A_1 A_2 \cdots A_n)^{1/n}} : A_{i+1} \geq \frac{3}{4} A_i, A_{i+2} \geq \frac{2}{3} A_i, \right\}
\]

(2), (3), \( A_1 = 1 \)

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<th>( n )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
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<td>4/3</td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>64/3</td>
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<td>256</td>
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<tr>
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<td>4/3</td>
<td>2</td>
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<td>21.3336</td>
<td>64.0012</td>
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Part III
Semidefinite Programming and Branch and Bound
Optimization

\[
\min \sum c_i A_i \\
\text{s.t. } A_i \text{ from KZ-reduced form} \\
A_n = 1
\]
PSD matrices

\[ q(x) = A_1(x_1 - \sum \alpha_{1j}x_j)^2 + \cdots + A_n x_n^2 \]

\[
\begin{align*}
Q &= Q^1 + \begin{array}{c}
0 \\| Q^2 \\
Q^2 & Q^n
\end{array} + \cdots + 0
\end{align*}
\]
SDP

\[
\min \sum c_i Q_{11}^i \\
\text{s.t.} \quad Q_i \text{ has rank 1} \\
Q_i \succeq 0 \\
d_1^T Q_i d_2 \geq 0 \text{ for all } d_1, d_2 \in D_i \\
Q_{11}^i \leq \sum_{k=i}^{n} x^T Q^k x \text{ for all } x \in \mathbb{Z}^{n-i+1}
\]

where \( D_i \) encodes \(|\alpha_{ij}| \leq 1/2\)
Novikova’s result

\[ q(x) = A_1(x_1 - \sum \alpha_{1j}x_j)^2 + \cdots + A_nx_n^2 \]

**Theorem (Novikova 1983).**
Finite check, independent of \( q \), to verify if \( q(x) \) is KZ-reduced.
SDP

$$\begin{align*}
\min & \quad \sum c_i Q_{11}^i \\
\text{s.t.} & \quad Q^i \text{ has rank } 1 \\
& \quad Q^i \succeq 0 \\
& \quad d_1^T Q^i d_2 \geq 0 \text{ for all } d_1, d_2 \in D_i \\
& \quad Q_{11}^i \leq \sum_{k=i}^n x^T Q^k x \text{ for all } x \in \mathbb{Z}^{n-i+1}
\end{align*}$$

where $D_i$ encodes $|\alpha_{ij}| \leq 1/2$
SDP

$$\begin{align*}
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& \quad Q_{11}^i \leq \sum_{k=i}^{n} x^T Q^k x \text{ for all } x \in X_{n-i+1}
\end{align*}$$

(r) \quad (p) \quad (s) \quad (n)

where $D_i$ encodes $|\alpha_{ij}| \leq 1/2$
**SDP Relaxation**

\[
\begin{align*}
\text{min} & \quad \sum c_i Q^i_{11} \\
\text{s.t.} & \quad Q^i \succeq 0 \quad (p) \\
& \quad d_1^T Q^i d_2 \geq 0 \text{ for all } d_1, d_2 \in D_i \quad (s) \\
& \quad Q^i_{11} \leq \sum_{k=i}^{n} x^T Q^k x \text{ for all } x \in X_{n-i+1} \quad (n)
\end{align*}
\]

where \( D_i \) encodes \(|\alpha_{ij}| \leq 1/2\)
Branch and bound
Implementation notes

• Compute rank-1 solution “close to” result
• Determine interval to split
• Dual problem gives lower bound
• Round to rational for rigorous proof (ε loss)
• Problem: numerical stability
Part IV
Future Work
Conjectures
Theorem (Pendavingh, vZ 2007).

\[-25A_1 - 36A_2 + 48A_3 + 40A_4 \geq -7 \cdot 10^{-6} A_4\]
\[-5A_1 + 2A_4 + 8A_5 \geq -3 \cdot 10^{-4} A_5\]
\[-4A_1 - 3A_3 + 4A_4 + 8A_5 \geq -5 \cdot 10^{-5} A_5\]
Conjectures

Conjecture (Pendavingh, vZ 2007).

\[-25A_1 - 36A_2 + 48A_3 + 40A_4 \geq 0\]
\[-5A_1 + 2A_4 + 8A_5 \geq 0\]
\[-4A_1 - 3A_3 + 4A_4 + 8A_5 \geq 0\]
Untried approaches

• Lasserre’s method (exploit sparsity)
• Cutting planes
• Newer solvers
• Extract rank-1 solutions (interesting lattices!)
Open problems

- Determine cone of outer coefficients for $n \geq 5$
- Improve the bound for $n \geq 9$
- Find an easier proof for $n \leq 8$

Modest goal

Problem.
Show that, for $n = 10$, a non-lattice packing has density higher than any lattice packing
Slides, paper at http://www.cwi.nl/~zwam/
Programs, data at http://www.win.tue.nl/kz/
The End