Limitations from Modular Forms on LP-Bounds for Sphere Packing

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Abstract

In 2016, Vizovska proved that the E_8 lattice gives the densest sphere packing problem in 8-dimesions [1]. Shortly thereafter, Cohn, Kumar, Miller, Radchenko, and Viazovska proved that the Leech lattice gives the densest sphere packing in 24-dimensions [2]. Their proofs find feasible solutions to the the Cohn-Elkies LP-method [3] to give upper bounds on the density of sphere packings in 8 and 24 dimensions that match sphere packings centered on the E_8 and Leech lattice respectively.

We prove that in contrast to the situation in dimensions 8 and 24, the LP-method is insufficient to prove that the densest known sphere packing is indeed the densest sphere packing in 12 and 16 dimensions. We also provide evidence that the same is true in dimensions $20, 28, 32$, and 36. The obstructions comes from modular forms. Moreover, we describe a general method involving linear programming over spaces of modular forms which appears to be the obstruction making the LP-method insufficient to solve the sphere packing problem in a wide range of dimensions.

Sphere Packing Definitions/Notation

- A *sphere packing* $\mathcal{P}$ in $\mathbb{R}^d$ is a disjoint union of open unit balls $\bigcup_{p\in P} B(p,1)$ for some subset $P \subset \mathbb{R}^d$.
- The *upper density* of a sphere packing $\mathcal{P}$ is defined to be
$$\Delta_{\mathcal{P}} := \limsup_{r\to\infty} \sup_{p\in\mathbb{R}^n} \frac{\mathrm{vol}(B(p,r)\cap\mathcal{P})}{\mathrm{vol}(B(p,r))}.$$
- The *sphere packing constant* (in dimension d) is
$$\Delta(:= \Delta_d) := \sup_{\substack{\mathcal{P}\subset\mathbb{R}^n \\ \text{Sphere Packing}}} \Delta_{\mathcal{P}}.$$
- The *center density*
$$\delta_{\mathcal{P}} := \frac{\Delta_{\mathcal{P}}}{B(0,1)} = \limsup_{r\to\infty} \sup_{p\in\mathbb{R}^n} \frac{\#(B(p,r)\cap P)}{\mathrm{vol}(B(p,r))},$$
measures the number of center points per unit volume of a packing.

Analytic Definitions/Notation

- $J_{\frac{d}{2}-1}$ is the *Bessel function of the first kind of order* $\frac{d}{2}-1$.
- Given function $f:\mathbb{R}\to\mathbb{R}$, define the *$d$-dimensional radial Fourier transform* by
$$\hat{f}(t) := \frac{(2\pi)^{d/2}}{k^{(d-2)/2}} \int_0^\infty x^{\frac{d}{2}} f(x) J_{\frac{d-2}{2}}(xt)\,dx$$
if the integral converges. If we set $F:\mathbb{R}^d\to\mathbb{R}$ and $\hat{F}:\mathbb{R}^d\to\mathbb{R}$ by $F(x) = f(|x|)$ and $\hat{F}(t) = \hat{f}(|t|)$, then $\hat{F}$ is the usual Fourier transform of F.
- A function $f:\mathbb{R}\to\mathbb{R}$ is *admissible* if there is a constant $\epsilon > 0$ such that both $|f(x)|$ and $|\hat{f}(x)|$ are $O(n^{-d-\epsilon})$.
- δ_x denotes a point mass at x.

Modular Forms Definitions/Notation

- We denote the upper half plane by
$$\mathcal{H} := \{z\in\mathbb{C} : \mathrm{im}(z) > 0\}.$$
- Define the congruence subgroup $\Gamma_0(N)$ by
$$\Gamma_0(N) := \left\{\begin{pmatrix} a & b \\ c & d\end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}) : c \equiv 0 \mod N\right\}$$
- Given a matrix
$$\gamma := \begin{pmatrix} a & b \\ c & d\end{pmatrix},$$
and an integer k, define the *slash operator* on functions $g:\mathcal{H}\to\mathbb{C}$ by
$$g|_{k,\gamma}(z) := \frac{(\det\gamma)^{k/2}}{(cz+d)^k} g\left(\frac{az+b}{cz+d}\right).$$
- The space $M_k(N) = M_k(\Gamma_0(N))$ of modular forms of weight k and level N is defined to be the set of functions $g:\mathcal{H}\to\mathbb{C}$ such that
$$g|_\gamma(z) = g(z) \text{ for all } \gamma\in\Gamma_0(N).$$
- Any $g\in M_k(N)$ has a q-expansion of the form $\sum_{n=0}^\infty a_n q^n$.
- $E_k(N)$ denotes the set of *Eisenstein series* of weight k and level $\Gamma_0(N)$. The Eisenstein series have q-expansions
$$E_t^\phi := \frac{\delta(\phi)}{2} L(1-k,\overline{\phi}) + \sum_{n=1}^\infty \sigma_{k-1}^{\phi,\overline{\phi}}(n) q^{tn},$$
where $u^2t|N$,
$$\phi:\mathbb{Z}\to(\mathbb{Z}/u\mathbb{Z})^\times\cup\{0\}\to\mathbb{C}$$
is a primitive Dirichlet character for u extended to a map from $\mathbb{Z}$ to $\mathbb{C}$, and
$$\sigma_{k-1}^{\phi,\overline{\phi}}(x) := \begin{cases} \sum_{\substack{m|x,\\ m>0}} \phi(x/m)\overline{\phi}(m) m^{k-1} & \text{if } x\in\mathbb{Z}, \\ 0 & \text{if } x\notin\mathbb{Z}.\end{cases}$$
Moreover, there is a unique Eisenstein series for each pair (ϕ,t) and these series are linearly independent.
- Let $\mathcal{E}_k(N)$ be the span of $E_k(N)$.
- A modular form is *cuspidal* (a *cusp form*) if it vanishes at all of the cusps of $\Gamma_0(N)\backslash\mathcal{H}$. The space of cusp forms is $S_k(N)$.
- Let $C_k(N)$ be the basis of $S_k(N)$ consisting of simultaneous Hecke eigenforms normalized so that the first non-zero coefficient of the q-expansion is equal to 1.

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Main Result: LP Method Cannot Prove Densest Known Packing is Optimal for $d\in\{12,16\}$.

Dimension	Largest Known $\delta_{\mathcal{P}}$	New Lower Bound to LP	LP Upper Bound	N	k	T
8	0.0625		0.0625	1	4	1
12	0.03704	0.05978	0.06279	24	6	4
12	0.03704	≈ 0.062319	0.06279	192	6	34
16	0.0625	0.10394	0.10738	24	8	6
20	0.13154	≈ 0.25786	0.27855	24	10	9
24	1.0		1.0	1	12	2
28	1.0	≈ 4.57598	5.02059	24	14	9
32	2.5658	≈ 28.08588	32.06222	24	16	12
36	4.4394	≈ 214.5447	258.54994	24	18	11

Table 1: Best lower bounds to the LP method in various dimensions. The exact bounds in dimensions 12 and 16 come from running Algorithm 1 using the PPL LP solver in Sage. Bounds marked with $\approx$ have not yet been proved, but were identified running Step 2 of Algorithm 1 using the approximate LP solver GLPK. In these cases, it is likely that our algorithm would give a slightly lower bound if run with an exact LP solver. The bound is proved by constructing a suitable modular form $f\in M_k(\Gamma_0(N))$ such that the first non-zero coefficient after a_0 in the q-expansion of f is a_T. In particular, the second and fourth rows certify that the LP method is insufficient to prove that the densest known sphere packings in 12 and 16 dimensions are actually the densest sphere packings in those dimensions.

Introduction to the LP Method

The LP Method, developed by Cohn and Elkies in [3] uses linear programming to prove upper bounds on the density of sphere packings. It is the source of the best known upper bounds for the center density of sphere packings in dimensions 4 through 36. The method was used to prove that the E_8 and Leech lattices yield optimal sphere packings in dimensions 8 and 24 respectively.

The LP Method upper bounds the density of sphere packing in dimension d by solving the following optimization problem.

Problem 1.

$$\begin{aligned} &\text{minimize} && \frac{f(0)}{\hat{f}(0)}\cdot\frac{r^d}{2^d} = \left(\sqrt[d]{\frac{f(0)}{\hat{f}(0)}}\cdot\frac{r}{2}\right)^d \\ &\text{subject to} && f:\mathbb{R}\to\mathbb{R} \text{ is an admissible function} && (1.\text{i}) \\ &&& f(0) > 0 && (1.\text{ii}) \\ &&& \hat{f}(0) > 0 && (1.\text{iii}) \\ &&& f(x)\le 0 \text{ for } |x|\ge r && (1.\text{iv}) \\ &&& \hat{f}(t)\ge 0 \text{ for all } t && (1.\text{v}).\end{aligned}$$

Theorem 1 (Cohn-Elkies [3]).
Let X be the optimal value for Problem 1. Then, $X\ge\delta_{\mathcal{P}}$ for any sphere packing $\mathcal{P}\subset\mathbb{R}^d$.

Remark.
While the objective function of Problem 1 is non-linear, it is invariant under scaling the input to f. Normalizing f by fixing the value of $\frac{f(0)}{\hat{f}(0)}$ and linearizing the objective function by replacing it with its dth root gives a linear program. Alternately, normalizing f by fixing r gives a different linear program.

A Dual to Problem 1

The standard approach for bounding linear programs is to consider the dual problem. The dual to Problem 1 is essentially Problem 2.

Problem 2.

$$\begin{aligned} &\text{maximize} && \frac{b_0}{a_0}\frac{R^d}{2^d} = \left(\sqrt[d]{\frac{b_0}{a_0}}\frac{R}{2}\right)^d \\ &\text{subject to} && \mu_1 \text{ and } \mu_2 \text{ are measures on } \mathbb{R}, && (2.\text{i}) \\ &&& a_0, b_0, R > 0 \text{ are real numbers}, && (2.\text{ii}) \\ &&& \mu_1 - a_0\delta_0 \text{ and } \mu_2 - b_0\delta_0 \text{ are positive measures}, && (2.\text{iii}) \\ &&& \mu_1 - a_0\delta_0 \text{ is identically zero on } \{x : |x| < R\}, && (2.\text{iv}) \\ &&& \textstyle\int_{\mathbb{R}} f(x)\mu_1 = \int_{\mathbb{R}} \hat{f}(t)\mu_2 \text{ for all } f \text{ admissible}. && (2.\text{v})\end{aligned}$$

Remark.
As with Problem 1, Problem 2 is invariant under scaling and gives rise to two distinct linear programs. In this project, we study the case where R is fixed.

Proposition 2.
Let X and Y be feasible values for Problem 1 and 2 respectively. Then, $Y\le X$.

Proof.
Scaling f, μ_1 and μ_2, we may assume $r = R = 1$. Then,
$$\frac{f(0)}{\hat{f}(0)} \ge \frac{1}{a_0\hat{f}(0)}\int_0^\infty f(x)\mu_1 = \frac{1}{a_0\hat{f}(0)}\int_0^\infty \hat{f}(t)\mu_2 \ge \frac{b_0}{a_0}.$$

Why Good Lower Bounds Are Hard to Find

- Constructing distributions which are identically zero on an interval $(0,R)$ and satisfy positivity conditions on the Fourier transform is difficult.
- Testing whether general measures are positive is difficult and cannot readily be implemented with off-the-shelf LP solvers.

Restricting to Measures with Discrete Support

Optimizing over spaces of μ_1 and μ_2 which are discretely supported solves many of the computational challenges in Problem 2. We consider the case where μ_1 and μ_2 are sums of δ-functionals.

Let $\{x(n)\}_{n=0}^\infty$ and $\{t(n)\}_{n=0}^\infty$ be increasing sequences with $x(0) = t(0) = 0$ and consider μ_1 and μ_2 of the form
$$(\mu_1,\mu_2) = \left(\sum_{n=0}^\infty a_n\delta_{x(n)}, \sum_{n=0}^\infty b_n\delta_{t(n)}\right).$$
Problem 2 restricts to

Problem 3.

$$\begin{aligned} &\text{maximize} && \frac{b_0}{a_0}\frac{R^d}{2^d} = \left(\sqrt[d]{\frac{b_0}{a_0}}\frac{R}{2}\right)^d \\ &\text{subject to} && a_0, b_0, R > 0 \text{ are real numbers}, && (3.\text{i}) \\ &&& a_n = 0 \text{ when } 0 < x(n) < R, && (3.\text{ii}) \\ &&& a_n, b_n \ge 0 \text{ for all } n, && (3.\text{iii}) \\ &&& \sum_{n=0}^\infty a_n f(x(n)) = \sum_{n=0}^\infty b_n\hat{f}(t(n)) \text{ for } f \text{ admissible}. && (3.\text{iv})\end{aligned}$$

In particular, any lower bound for Problem 3 is a lower bound for Problems 1 and 2.

An Algorithm for Bounding the LP Method

We assume that N is not divisible by 16^2, 9^2 or p^2 for any prime $p > 3$. This guarantees that $M_k(N)$ has a basis of forms (extending the set of Eisenstein series) with all real coefficients.

Let
$$\{g^1,\ldots,g^{\dim M_k(N)}\}$$
be such a basis of $M_k(N)$. Let $h^j := i^k g^j|_{W_n}$ be i^k times the image of g^j under the full level N Atkin-Lehner involution. Write the q-expansions of the h^j and g^j as
$$g^j := \sum_{n=0}^\infty a_n^j q^n \qquad h^j := \sum_{n=0}^\infty b_n^j q^n.$$
Fix integers T and M with $1\le T < \dim M_k(N) < M$.

Algorithm 1:
Input: $k = d/2$ with $2|k$, a positive integer N which is not divisible by 16^2, 9^2 or p^2 for any prime $p > 3$ and integers T, M satifying $1\le T < \dim M_k(N) < M$.
Output: Either returns a value X which is a lower bound for the optimal value of Problems 1 and 2, or returns fail.

1. Compute the q-expansions of a basis for the space of modular forms of weight k and level N up to precision M.
2. Solve the following linear program:
Problem 4.
$$\begin{aligned} &\text{maximize} && \textstyle\sum x_j b_0^j \\ &\text{subject to} && 1 = \textstyle\sum x_j a_0^j && (3.\text{i}) \\ &&& 0 = \textstyle\sum x_j a_n^j \text{ for } 1\le n < T && (3.\text{ii}) \\ &&& 0 \le \textstyle\sum x_j a_n^j \text{ for } T\le n\le M && (3.\text{iii}) \\ &&& 0 \le \textstyle\sum x_j b_n^j \text{ for } 1\le n\le M && (3.\text{iv})\end{aligned}$$
3. Given a feasible solution to Problem 4, let $g = \sum x_j g^j$ and $h = \sum x_j h^j$. Check that all of the coefficients of the q-expansions of g and h are non-negative.
4. If this check fails, return fail. If this check succeeds, return $X := (\sum x_j b_0^j)\cdot\left(\frac{T}{2N}\right)^{d/2}$.

If the algorithm fails in step 4, one can increase M and attempt the optimization problem again. In practice, $M = 2\cdot\dim M_k(N)$ typically seems to be sufficient for the algorithm to succeed.

Main Theorem

Theorem 3.
Algorithm 1 (above) is correct and runs in finite time.

Proof.
Proposition 4 says that Problem 4 is a relaxation of Problem 3 with $x(n) = \sqrt{n}$ and $t(n) = 2\sqrt{n/N}$. The only missing condition is (3.iii) for $n > M$. The coefficients of the modular forms are rational, so equality conditions can be checked precisely by computer. The check in Step 3 certifies that (3.iii) holds or returns fail if it does not. This proves correctness.
Computing truncated q-expansions, solving finite-dimensional linear programs and the positivity check laid out in the right-hand column are finite-time, so Algorithm 1 is finite-time.

Algorithm 1 in Practice/Next Steps

- Numerical precision is the biggest obstacle to running Algorithm 1 in practice. Cusp forms coefficients grow much more slowly than Eisenstein series coefficients, so LP solvers overflow on moderate parameters. A quad precision solver would give stronger results.
- Truncating computation time would give results for more d.
- In the next code rewrite, Algorithm 1 will be reorganized to more easily extract exact bounds from an approximate LP solver.
- Algorithm 1 can be modified to apply when N is divisible by larger squares, with modular forms of nontrivial nebentype, and/or with sums twisted by Dirichlet characters. In these cases, we expect that the space of forms with positive real coefficients is relatively small. We hope to investigate this in future work.
- We hope to relate this approach to the constructions in [1] and [2] to nail down best possible LP bounds in many dimensions.

For More Information

- For a preprint or code, email ngtriant@mit.edu.
- This poster will be available at
`http://www-math.mit.edu/~ngtriant/research.html`

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An Analogue of Poisson/Voronoi Summation

Algorithm 1 depends on the following summation forumula, which is analogous to the Poisson and Voronoi summation formulas.

Proposition 4.

- Let $d = 2k$ for $k\in\mathbb{Z}$.
- Let $g\in M_k(\Gamma_0(N))$ be a modular form of weight k and level $\Gamma_0(N)$.
- Let $w_N = \begin{pmatrix} 0 & -1 \\ N & 0\end{pmatrix}$.
- Let
$$\tilde{g}(z) = g|_{w_N}(z) = \frac{i^k}{N^{k/2}z^k} g\left(-\frac{1}{Nz}\right)$$
be i^k times the image of g under the full level N Atkin-Lehner operator.
- Let the q-expansions of g and $\tilde{g}$ be
$$g(z) = \sum_{n=0}^\infty a_n q^n, \qquad \tilde{g}(z) = \sum_{n=0}^\infty b_n q^n.$$

Then,
$$\sum_{n=0}^\infty a_n f(\sqrt{n}) = \left(\frac{2}{\sqrt{N}}\right)^{d/2} \sum_{n=1}^\infty b_n\hat{f}\left(\frac{2\sqrt{n}}{\sqrt{N}}\right)$$
where $\hat{f}$ denotes the d-dimensional radial Fourier transform.

Proof Sketch.
The proof is essentially standard. It follows by rewriting the L-function associated to g via Mellin inversion, shifting the contour of integration from real part $d+\epsilon/2$ to $-\epsilon/2$, applying the functional equation for modular L-functions, changing variables to move the contour back, and undoing the Mellin inversion. The a_0 and b_0 terms arise from shifting the contour across possible poles.

Remark.
By adjusting the multiplicative constant appropriately, Proposition 4 can be generalized to the case of modular forms of any nebentype and/or to sums twisted by a Dirichlet character.

Checking Positivity of Modular Form Coefficients

Given a modular form $g\in M_k(N)$, Algorithm 1 requires us to verify whether all of the coefficients of the q-expansion of g and $\tilde{g}$ are non-negative.

We take the following five-step approach to check whether the coefficients of a given modular form g are non-negative.

1. Write $g = g_e + g_c$, where
$$g_e = e_0 + \sum_{n=1}^\infty e_n q^n \in \mathcal{E}_k(N)$$
is the Eisenstein part of g and
$$g_c = \sum_{n=1}^\infty c_n q^n \in S_k(N)$$
is the cuspidal part of g.
2. Express g_e as a linear combination of Eisenstein series and use explicit formulas to get a bound of the form
$$e_n \ge A\cdot\sigma_{k-1}(n) > An^{k-1}$$
for some constant $A\in\mathbb{R}$.
3. Express g_c as a linear combination of normalized eigenforms and use Deligne's Weil bounds to get a bound of the form
$$|c_n| \le B\sigma_0(n) n^{(k-1)/2} \le Bn^{k/2}.$$
for some constant $B\in\mathbb{R}$.
4. Compare An^{k-1} to $Bn^{k/2}$ to show that there is a $Q\in\mathbb{Z}$ such that $e_n + c_n \ge 0$ for all $n\ge Q$.
5. Explicitly compute the coefficients of g for $0\le n < Q$ to check $e_n + c_n \ge 0$ for all $n\ge 0$.

Positivity Check in Detail

Steps 1, 4, and **5** are straightforward using built-in functions in Magma and some linear algebra.

Step 3. Write g_c in the form
$$g_c = \sum_{h\in C_k(N)} y_h h.$$
As a consequence of Deligne's proof of the Weil conjectures [4], the coefficient of n in the q-expansion of h is bounded above by $\sigma_0(n)n^{(k-1)/2}$. By the triangle inequality, we may take
$$B = \sum_{h\in C_k(N)} y_h.$$

Step 2. For simplicity, we assume N is not divisible by 16^2, 9^2 or p^2 for any prime $p > 3$. In this case, if $u^2|N$, then $u|24$. In particular, ϕ is a real character for all $E_t^\phi\in E_k(N)$. In this case,
$$\phi(n/m)\overline{\phi}(m) = \phi(n)\overline{\phi}(m)^2 = \phi(n)$$
for all $m|n$ and for any $n\in\mathbb{Z}$, so
$$\sigma_{k-1}^{\phi,\overline{\phi}}(x) = \phi(x)\sigma_{k-1}(x)$$
and so
$$E_t^\phi := \frac{\delta(\phi)}{2}L(1-k,\overline{\phi}) + \sum_{n=1}^\infty \phi(n/t)\sigma_{k-1}(n/t)q^n.$$
There are constants x_t^ϕ such that
$$g_e := \sum_{t|N} \sum_{\substack{\phi \text{ prim. for } u \\ u^2t|N}} x_t^\phi E_t^\phi,$$
whence
$$e_n = \sum_{t|N}\left(\sum_{\substack{\phi \text{ prim. for } u \\ u^2t|N}} \phi(n/t)x_t^\phi\right)\sigma_{k-1}(n/t). \qquad (1)$$
For $n/t\in\mathbb{Z}$, we have the inequality
$$\frac{\sigma^{k-1}(n)}{\sigma_{k-1}(t)} \le \sigma^{k-1}(n/t) \le \frac{\sigma^{k-1}(n)}{t^{k-1}}.$$
Applying either the lower or upper bound based on whether the sum over ϕ in (1) is positive or negative, and summing over t gives
$$e_n \ge A_n\sigma_{k-1}^n$$
for some $A_n\in\mathbb{R}$. Now, A_n depends only on the $n \mod N$, so we may take
$$A := \min_{n\in\{1,\ldots,N\}} A_n.$$