# An Approach to the Dodecahedral Theorem Based on Bounds for Spherical Codes

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The dodecahedral theorem



Workshop on Optimization

- The dodecahedral theorem
- Pejes Tóth's proof scheme





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- Relationship to spherical codes





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- 4 Strengthened bounds for spherical codes





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The Voronoi cell associated with  $x_0 = 0$  induced by the points  $2\bar{x}_i$ , i = 1, ..., m is

$$V(\bar{x}_1,...,\bar{x}_m) = \{x \mid ||x|| \leq ||2\bar{x}_i - x||, i = 1,...,m\}$$
  
= \{x \cdot |\bar{x}\_i^T x \leq ||\bar{x}\_i||^2, i = 1,...,m\}.





#### Theorem (Dodecahedral conjecture; L. Fejes Tóth, 1943)

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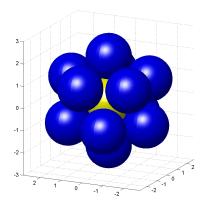
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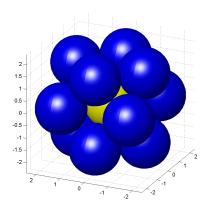




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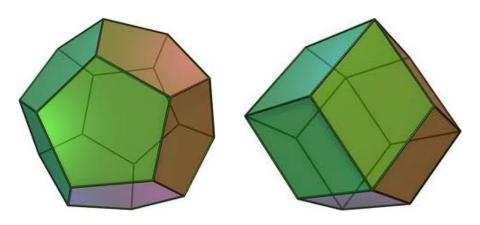


Figure: Regular and rhombic dodecahedra





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In his 1964 book *Regular Figures*, Fejes Tóth restates the dodecahedral conjecture and describes a scheme that would lead to a complete proof if a key inequality were established.





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Theorem (Fejes Tóth, 1964)

Let  $\hat{x}_i$ , i = 1, ..., m be points in  $\Re^3$  with  $\|\hat{x}_i\| \ge 1$  for each i. If  $m \le 12$ , then  $\operatorname{Vol}(V(\hat{x}_1, ..., \hat{x}_m) \cap \mathcal{B}_D) \ge \operatorname{Vol}(D)$ .





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Note that in the above theorem it is *not* assumed that the points satisfy  $\|\hat{x}_i - \hat{x}_j\| \ge 1$ ,  $i \ne j$ . Also, the assumption that  $\|\hat{x}_i\| < R_D$  for each i could be added, since if  $\|\hat{x}_i\| \ge R_D$  the constraint  $\hat{x}_i^T x \le \|\hat{x}_i\|^2$  does not eliminate any points in  $\mathcal{B}_D$ .





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For the Voronoi cell  $V(\hat{x}_1,\ldots,\hat{x}_m)$ , let  $F_i(\hat{x}_1,\ldots,\hat{x}_m)$  be the face of  $V(\hat{x}_1,\ldots,\hat{x}_m)\cap\mathcal{B}_D$  corresponding to the points with  $\hat{x}_i^Tx=\|\hat{x}_i\|^2$  (it is possible that  $F_i(\hat{x}_1,\ldots,\hat{x}_m)=\emptyset$ ).









Step 0. Input  $\bar{x}_i$ ,  $1 \le ||\bar{x}_i|| \le R_D$ , i = 1, ..., m with m > 12 and  $||\bar{x}_i - \bar{x}_i|| \ge 1$ ,  $i \ne j$ . Let  $\hat{x}_i = \bar{x}_i$ , i = 1, ..., m.





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- Step 1. If  $|\{i \mid 1 < \|\hat{x}_i\| < R_D\}| < 2$  then go to Step 3. Otherwise choose  $j \neq k$  such that  $1 < \|\hat{x}_j\| < R_D$ ,  $1 < \|\hat{x}_k\| < R_D$ , and the surface area of  $F_j(\hat{x}_1, \dots, \hat{x}_m)$  is less than or equal to that of  $F_k(\hat{x}_1, \dots, \hat{x}_m)$ .



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- Step 2. Let  $\delta = \min\{R_D \|\hat{x}_i\|, \|\hat{x}_k\| 1\}$ , and

$$\hat{x}_j \leftarrow (\|\hat{x}_j\| + \delta) \frac{\hat{x}_j}{\|\hat{x}_j\|}, \quad \hat{x}_k \leftarrow (\|\hat{x}_k\| - \delta) \frac{\hat{x}_k}{\|\hat{x}_k\|}.$$

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Step 3. Output  $\hat{x}_i$ , i = 1, ..., m.





Obvious that the adjustment in Step 2 leaves  $\sum_{i=1}^{m} \|\hat{x}_i\|$  unchanged, and can be shown that  $\operatorname{Vol}(V(\hat{x}_1,\ldots,\hat{x}_m)\cap\mathcal{B}_D)$  is nonincreasing. Note that adjustment in Step 2 is executed at most m-1 times, since each adjustment decreases  $|\{i \mid 1 < \|\hat{x}_i\| < R_D\}|$  by at least 1. At termination have at most one i with  $1 < \|\hat{x}_i\| < R_D$ .





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The previous theorem could then be applied to bound

$$\operatorname{Vol}(\textit{V}(\bar{\textit{x}}_1,\ldots,\bar{\textit{x}}_m)) \geq \operatorname{Vol}(\textit{V}(\bar{\textit{x}}_1,\ldots,\bar{\textit{x}}_m) \cap \mathcal{B}_{\textit{D}}) \geq \operatorname{Vol}(\textit{V}(\hat{\textit{x}}_1,\ldots,\hat{\textit{x}}_m) \cap \mathcal{B}_{\textit{D}})$$

if the  $\hat{x}_i$  output by the procedure have at most twelve i with  $\|\hat{x}_i\| < R_D$ . Note that the output points  $\hat{x}_i$  may *not* satisfy  $\|\hat{x}_i - \hat{x}_j\| \ge 1$ ,  $i \ne j$ , but this assumption is not required in the theorem.



This would be the case if the input points  $\bar{x}_i$  satisfy the key inequality

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Recall that have at most one i with  $1 < \|\hat{x}_i\| < R_D$ . Then if  $\|\hat{x}_i\| = 1$ ,  $i = 1, \ldots, 12$ , key inequality and the fact that  $\hat{x}_i \le R_D$  for each i together imply

$$(m-12)R_D \ge \sum_{i=13}^m \|\hat{x}_i\| \ge 12 + (m-12)R_D - 12 = (m-12)R_D,$$

so  $\|\hat{x}_i\| = R_D$  for i = 13, ..., m.





A complete proof of the dodecahedral conjecture thus requires only a proof that the key inequality holds for any  $\bar{x}_i$ ,  $i=1,\ldots,m$  with  $1 \leq \|\bar{x}_i\| \leq R_D$  for each i, and  $\|x_i - x_i\| \geq 1$  for all  $i \neq j$ .

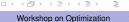




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Note key inequality for m=13 would give immediate proof of "Thirteen Spheres Problem."

# Theorem (13 spheres problem; Kissing number in dimension 3)

In a packing of unit spheres in  $\Re^3$ , at most 12 spheres can simultaneously touch ("kiss") another sphere.





To prove key inequality, need solution (or very good lower bound) for *m*-point norm minimization problem

min 
$$\sum_{i=1}^{m} ||x_i||$$
s.t. 
$$||\bar{x}_i - \bar{x}_j|| \ge 1, \quad i \ne j$$

$$1 \le ||\bar{x}_i|| \le R_D, \quad i = 1, \dots, m.$$

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Expect that these approaches may have difficulty due to number of variables (40-60), very high degree of symmetry, and need for a relatively tight bound. We will consider another possibility based on the theory of spherical codes.

#### **Outline**

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A set  $C = \{x_i\}_{i=1}^m \subset \Re^3$  is called a spherical *z*-code if  $||x_i|| = 1$  for each i, and  $x_i^T x_j \leq z$  for all  $i \neq j$ . A packing of unit spheres that all touch a unit sphere centered at the origin generates a spherical 1/2-code.





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To begin we establish that for R sufficiently small, if  $\{\bar{x}_i\}_{i=1}^m$  are points with  $1 \leq \|\bar{x}_i\| \leq R$  for each i and  $\|\bar{x}_i - \bar{x}_j\| \geq 1$  for all  $i \neq j$ , then the normalized points  $x_i = \bar{x}/\|\bar{x}_i\|$  form a z-code for a suitable z.





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# Lemma (Normalized points form spherical z-code)

Suppose that  $1 \le \|\bar{x}_i\| \le R$ , i = 1, ..., m, where  $R \le \frac{1+\sqrt{5}}{2} \approx 1.618$ and  $\|\bar{x}_i - \bar{x}_i\| \ge 1$  for all  $i \ne j$ . Let  $x_i = \bar{x}_i / \|\bar{x}_i\|$ ,  $i = 1, \ldots, m$ . Then  $x_i^T x_i \leq 1 - \frac{1}{2D^2}$  for all  $i \neq j$ .





Next, for  $x_i \neq x_i$  with  $||x_i|| = ||x_i|| = 1$ ,  $x_i^T x_i \leq 1 - \frac{1}{2R^2}$ ,  $R \leq \frac{1+\sqrt{5}}{2}$ , consider the 2-point norm minimization problem

min 
$$\lambda_i + \lambda_j$$
  
s.t.  $\|\lambda_i x_i - \lambda_j x_j\| \ge 1$   
 $1 \le \lambda_i \le R, \ 1 \le \lambda_j \le R.$ 





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# Theorem (Solution of 2-point norm minimization problem)

Let  $1 \le R \le \frac{1+\sqrt{5}}{2}$ ,  $||x_i|| = ||x_j|| = 1$  and  $.5 \le s = x_i^T x_j \le 1 - \frac{1}{2R^2}$ . Then problem solution has  $\lambda_i^* + \lambda_j^* = f(s,R)$ , where

$$f(s,R) = \begin{cases} 1 + 2s & \frac{1}{2} \le s \le \frac{R}{2}, \\ R(1+s) + \sqrt{1 - R^2(1-s^2)} & \frac{R}{2} \le s \le 1 - \frac{1}{2R^2}. \end{cases}$$





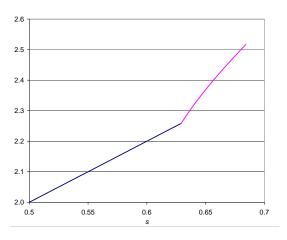


Figure: Solution value in 2-point norm minimization problem for  $R = R_D$ 



Now assume that m > 12,  $1 \le \|\bar{x}_i\| \le R_D$ ,  $i = 1, \dots m$ , and  $\|\bar{x}_i - \bar{x}_j\| \ge 1$  for all  $i \ne j$ . Let  $\lambda_i = \|\bar{x}_i\|$  and  $x_i = (1/\lambda_i)\bar{x}_i$ . Goal is to prove the key inequality, which can be written

$$\sum_{i=1}^{m} (\lambda_i - 1) \ge 12 + (m-12)R_D - m = (m-12)(R_D - 1).$$





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Define  $N_i = |\{j \neq i \mid x_i^T x_j \geq .5\}|$  to be the number of "close neighbors" of  $x_i$ , and  $\mathcal{N} = \{(i, j), i \neq j \mid x_i^T x_j \geq .5\}$ . Then  $|\mathcal{N}| = \sum_{i=1}^m N_i$ , and

$$\sum_{(i,j)\in\mathcal{N}} (\lambda_i + \lambda_j - 2) = \sum_{(i,j)\in\mathcal{N}} (\lambda_i - 1) + (\lambda_j - 1) = 2\sum_{i=1}^m N_i(\lambda_i - 1).$$





Applying the solution of the 2-point norm minimization problem, get

$$2\sum_{i=1}^{m} N_i(\lambda_i - 1) \geq \sum_{(i,j) \in \mathcal{N}} [f(x_i^T x_j, R_D) - 2]$$
$$\sum_{i=1}^{m} (\lambda_i - 1) \geq \frac{1}{2N_{\text{max}}} \sum_{(i,j) \in \mathcal{N}} [f(x_i^T x_j, R_D) - 2],$$

where  $N_{\text{max}} := \max\{N_i\}_{i=1}^m$ .





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$$\frac{1}{2N_{\max}} \sum_{(i,j) \in \mathcal{N}} [f(x_i^T x_j, R_D) - 2] \ge (m - 12)(R_D - 1).$$





Using results from spherical trigonometry, can prove

Lemma (Maximum number of close neighbors)

 $N_{\text{max}} \leq 6$ . Moreover, for m = 13, if  $N_{\text{max}} = 6$  then key inequality holds.





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# Lemma (Maximum number of close neighbors)

 $N_{\text{max}} \leq 6$ . Moreover, for m = 13, if  $N_{\text{max}} = 6$  then key inequality holds.

To get lower bound for

$$\frac{1}{2N_{\text{max}}}\sum_{(i,j)\in\mathcal{N}}[f(x_i^Tx_j,R_D)-2]$$

can apply Delsarte bound for spherical codes. Recall  $C = \{x_i\}_{i=1}^m$  is a spherical z-code in  $\Re^3$ , with  $z = 1 - 1/(2R_D^2) \approx .6843$ .





For  $\alpha \in [-1, 1]$ , define the distance distribution of the code to be

$$\alpha(s) = \frac{|\{(i,j) \mid x_i^T x_j = s\}|}{m}.$$

Then  $\alpha(\cdot) \ge 0$ , and  $\sum_{-1 \le s \le z} \alpha(s) = m - 1$ .





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Let  $\Phi_k(\cdot)$ ,  $k=0,1,\ldots$  denote the Gegenbauer, or ultraspherical, polynomials  $\Phi_k(t) = P_k^{(0,0)}(t)$  where  $P_k^{(0,0)}$  is a normalized Jacobi polynomial. It can be shown that

$$1 + \sum_{-1 \le s \le z} \alpha(s) \Phi_k(s) \ge 0, \quad k = 1, 2, \dots$$

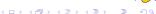




Then  $\sum_{(i,j)\in\mathcal{N}}[f(x_i^Tx_j,R_D)-2] \geq v^*(m)$ , where  $v^*(m)$  is solution value in the semi-infinite LP problem

LP(
$$m$$
): min  $m \sum_{.5 \le s \le z} [f(s, R_D) - 2] \alpha(s)$   
s.t.  $\sum_{-1 \le s \le z} \alpha(s) \Phi_k(s) \ge -1, \quad k = 1, \dots, d$   
 $\sum_{-1 \le s \le z} \alpha(s) = m - 1$   
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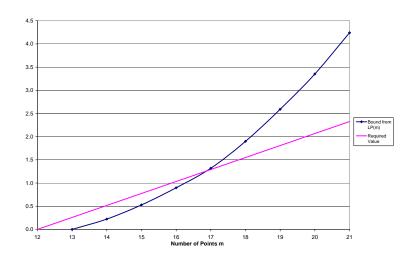
LP(
$$m$$
):  $\min m \sum_{0.5 \le s \le z} [f(s, R_D) - 2] \alpha(s)$   
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Constraints of LP(m) are feasible up to m = 21. To establish key inequality, need

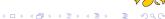
$$v^*(m)/(2N_{\text{max}}) \ge (m-12)(R_D-1), \qquad m=13,\ldots,21.$$











**Result:** Bound from LP(m) sufficient to prove key inequality for  $m \ge 17$ . Remains to prove inequality for m = 13, ..., 16.



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Note  $v^*(13) = 0$ . In fact knew this would be the case ahead of time, since Delsarte bound for kissing number in dimension 3 is 13, not 12. Need to strengthen Delsarte bound to have any chance of proving key inequality for m = 13.



### **Outline**

- The dodecahedral theorem
- Pejes Tóth's proof scheme
- Relationship to spherical codes
- Strengthened bounds for spherical codes







• A (2003)





- A (2003)
- Musin (2003)





- A (2003)
- Musin (2003)
- Bachoc and Vallentin (2007)





- A (2003)
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All three are sufficient to prove that kissing number in dimension 3 is 12. Last approach is most powerful and results in SDP in place of LP.





#### Resulting problem SDP(m) has form:

$$\min \quad m \sum_{.5 \le s \le z} [f(s, R_D) - 2] \alpha(s)$$

s.t. 
$$\sum_{s \in Z} \alpha(s) \Phi_k(s) \ge -1, \quad k = 1, \dots, d$$
$$\sum_{s \in Z} \alpha(s) = m - 1, \quad \alpha(s) \ge 0, \quad s \in Z = [-1, z]$$





#### Resulting problem SDP(m) has form:

$$\begin{aligned} & \min \quad m \sum_{.5 \le s \le z} [f(s,R_D) - 2] \alpha(s) \\ & \text{s.t.} \quad \sum_{s \in Z} \alpha(s) \Phi_k(s) \ge -1, \quad k = 1, \dots, d \\ & \sum_{s \in Z} \alpha(s) = m - 1, \quad \alpha(s) \ge 0, \quad s \in Z = [-1,z] \\ & 3 \sum_{s \in Z} \alpha(s) S_k(s,s,1) + \sum_{s,t,u \in Z} \alpha'(s,t,u) S_k(s,t,u) \succeq -S_k(1,1,1), \\ & \qquad k = 1, \dots, d \\ & \sum_{s,t,u \in Z} \alpha'(s,t,u) \ge 0, \quad s,t,u \in Z. \end{aligned}$$





In SDP(m),  $\alpha'(\cdot, \cdot, \cdot)$  is the 3-point distance distribution

$$\alpha'(s,t,u) = \frac{\left|\left\{\left(i,j,k\right) \mid x_i^T x_j = s, x_i^T x_k = t, x_j^T x_k = u\right\}\right|}{m}$$

and  $S_k(s, t, u)$  is a  $(d + 1 - k) \times (d + 1 - k)$  symmetric matrix whose entries are symmetric polynomials of degree k in the variables (s, t, u)





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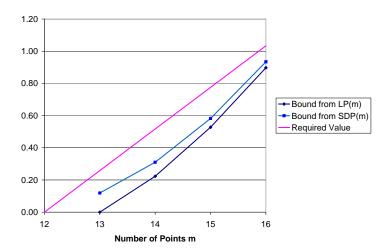
$$\alpha'(s,t,u) = \frac{\left|\left\{\left(i,j,k\right) \mid x_i^T x_j = s, x_i^T x_k = t, x_j^T x_k = u\right\}\right|}{m},$$

and  $S_k(s, t, u)$  is a  $(d + 1 - k) \times (d + 1 - k)$  symmetric matrix whose entries are symmetric polynomials of degree k in the variables (s, t, u)

Can also add constraints relating 2-point and 3-point distance distributions and remove original constraints based on  $\Phi_k(\cdot)$ .













 Can add constraints on 3-point distance distribution based on spherical Delaunay triangulation.



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# Thank You!



