

ICERM Conference on  
Computational Challenges in the Theory of Lattices  
Providence, April 2018

# Variations and Applications of Voronoi's algorithm

Achill Schürmann  
(Universität Rostock)

( based on work with Mathieu Dutour Sikiric and Frank Vallentin )

PRELUDE

Voronoi's Algorithm

- classically -

# Lattices and Quadratic Forms

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- Every **lattice basis**  $A \in \text{GL}_n(\mathbb{R})$  of a lattice  $L = A\mathbb{Z}^n$  defines a **positive definite symmetric (Gram) matrix**  $Q = A^t A$ .

$$\mathcal{S}_{>0}^n := \{ Q \in \mathbb{R}^{n \times n} : Q \text{ symmetric and positive definite} \}$$

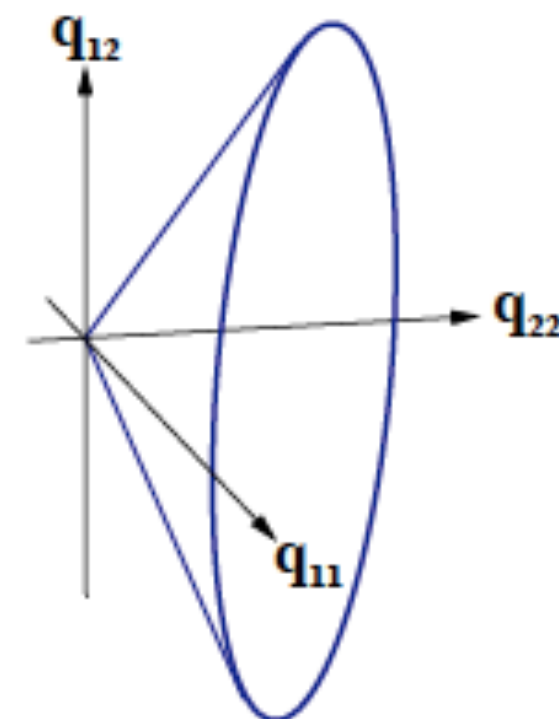
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- $Q \in \mathcal{S}_{>0}^n$  defines a **pos. def. quadratic form (PQF)**

$$Q[x] = x^t Q x = \sum_{i=1}^n q_{ii} x_i^2 + 2 \sum_{i < j} q_{ij} x_i x_j$$



Different bases of a lattice yield **integrally equivalent** PQFs:

$$L = A\mathbb{Z}^n \Leftrightarrow L = (AU)\mathbb{Z}^n \text{ for } U \in \text{GL}_n(\mathbb{Z})$$

$$A^t A = Q \sim Q' = U^t Q U = (AU)^t (AU)$$

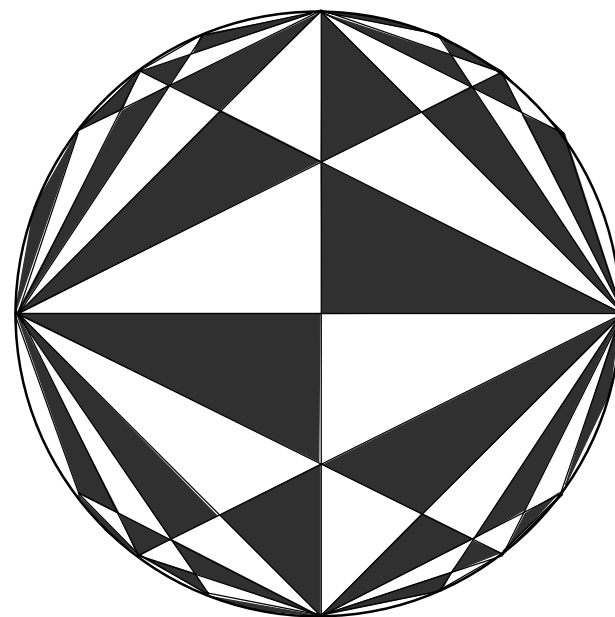
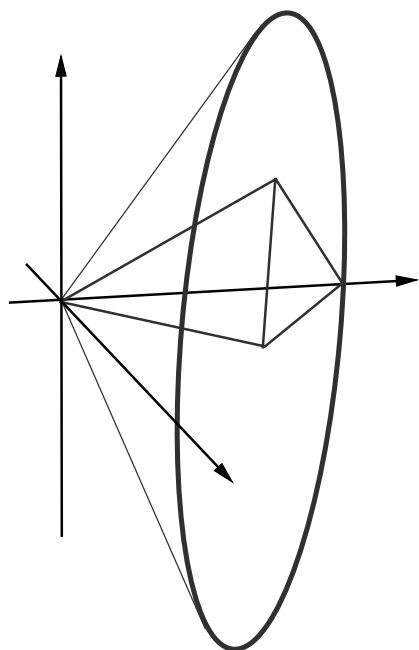
# Reduction Theory

for positive definite quadratic forms

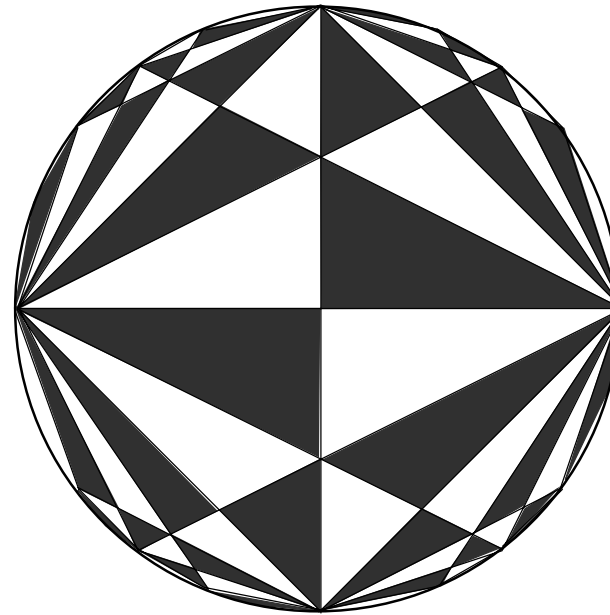
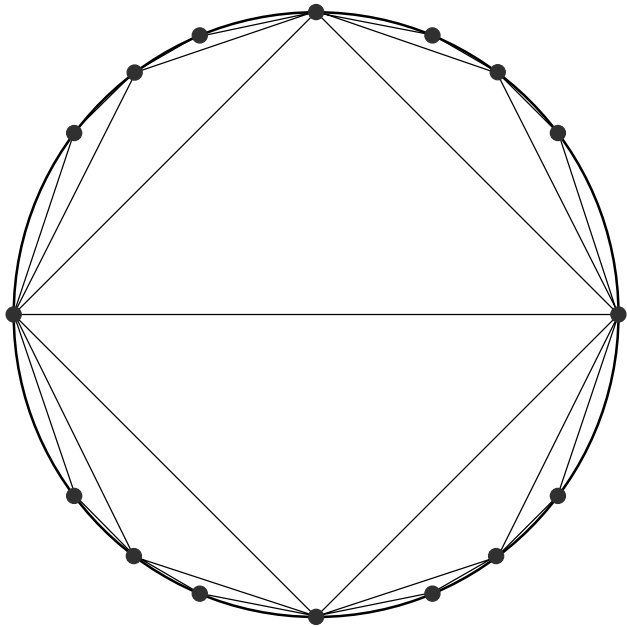
$\mathrm{GL}_n(\mathbb{Z})$  acts on  $\mathcal{S}_{>0}^n$  by  $Q \mapsto U^t Q U$

Task of a **reduction theory** is to provide a **fundamental domain**

Classical reductions were obtained by Lagrange, Gauß, Korkin and Zolotareff, Minkowski and others... All the same for  $n = 2$ :



# Voronoi's reduction idea



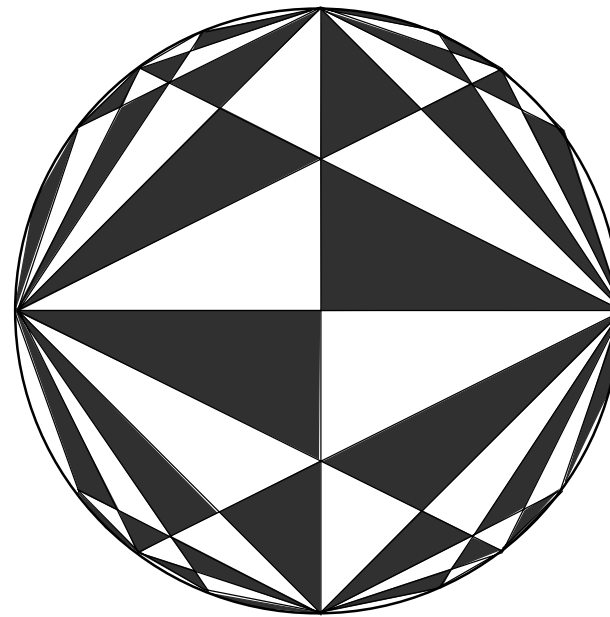
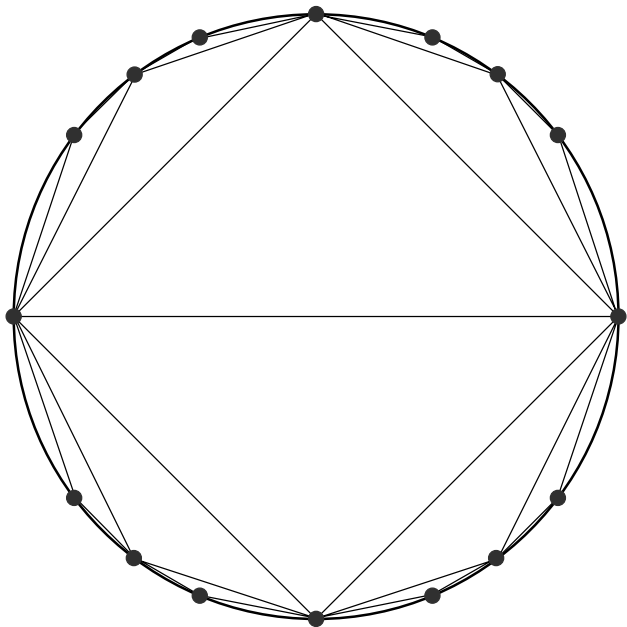
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**Observation:** The fundamental domain can be obtained from polyhedral cones that are spanned by rank-1 forms only

**Voronoi's algorithm** gives a recipe for the construction of a complete list of such polyhedral cones up to  $GL_n(\mathbb{Z})$ -equivalence



# Perfect Forms

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(Voronoi cones are full dimensional if and only if  $Q$  is perfect!)

# Ryshkov Polyhedron

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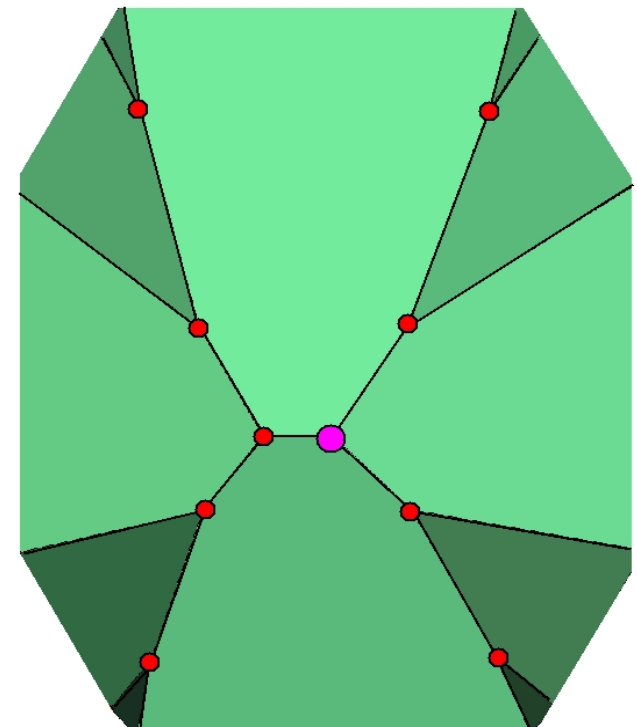
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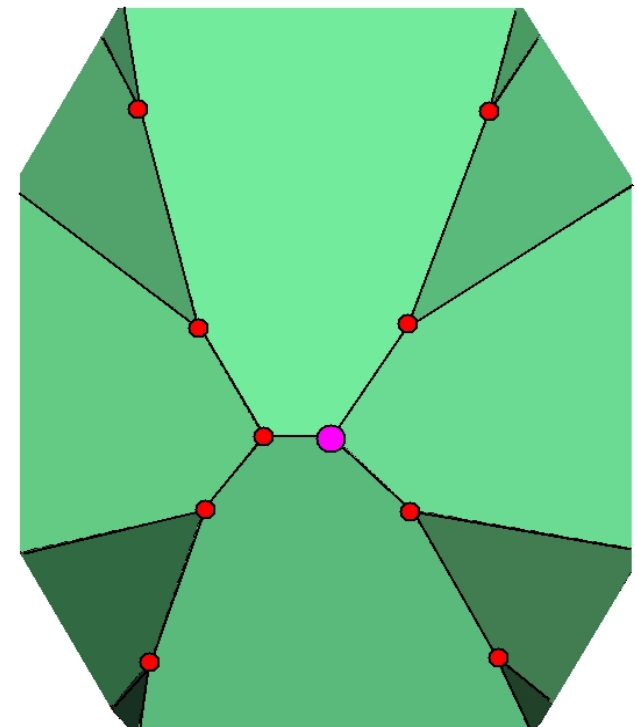
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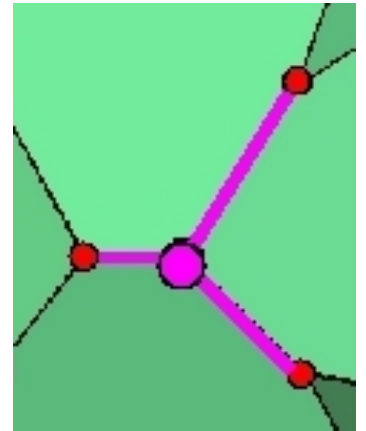
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- $\mathcal{R}$  is a **locally finite polyhedron**
- Vertices of  $\mathcal{R}$  are perfect



# Voronoi's Algorithm



Start with a perfect form  $Q$

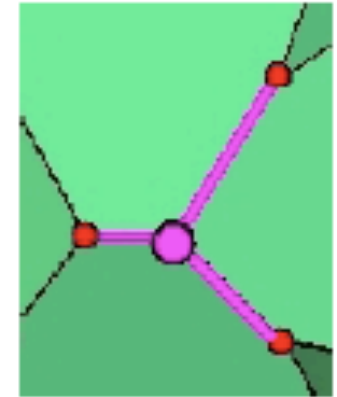
1. **SVP**: Compute  $\text{Min } Q$  and describing inequalities of the polyhedral cone

$$\mathcal{P}(Q) = \{ Q' \in \mathcal{S}^n : Q'[x] \geq 1 \text{ for all } x \in \text{Min } Q \}$$

2. **PolyRepConv**: Enumerate extreme rays  $R_1, \dots, R_k$  of  $\mathcal{P}(Q)$
3. **SVPs**: Determine contiguous perfect forms  $Q_i = Q + \alpha R_i, i = 1, \dots, k$
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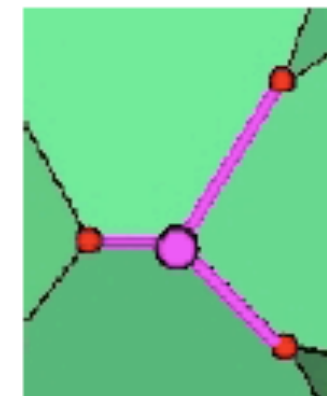
# Computational Results

- **BOTTLENECK:** Computing vertices of polyhedra!
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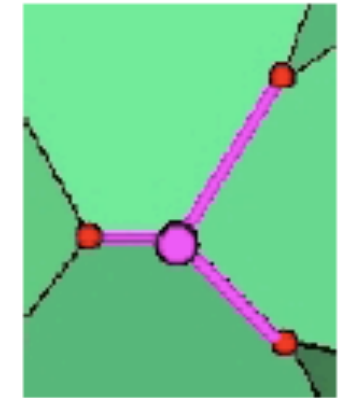
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**Computer assisted proof** with *Recursive Adj. Decomp. Method (ADM)*  
for vertex enumeration **up to symmetries**

( showing that the “ $E_8$ -polytope” has 25075566937584 vertices in 83092 orbits )

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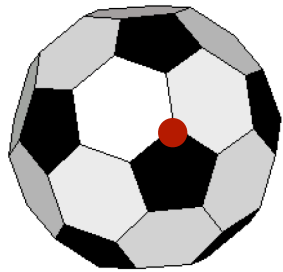
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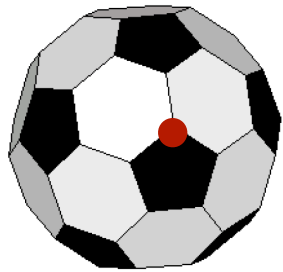


- Find initial orbit(s) / representing vertice(s)

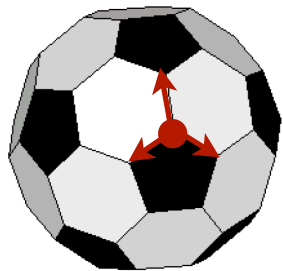


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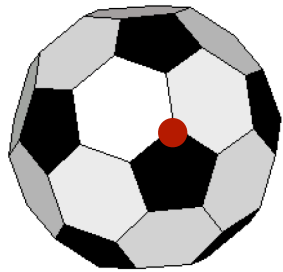
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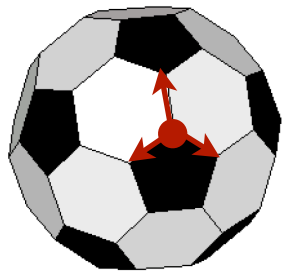
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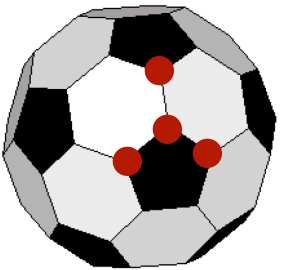
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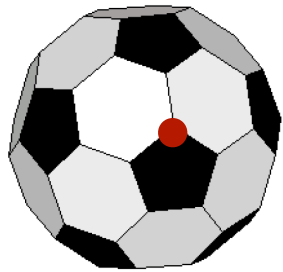
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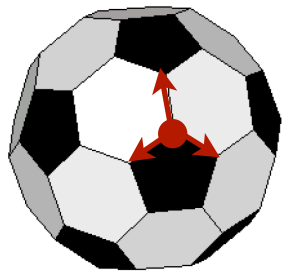
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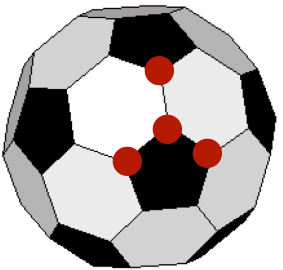
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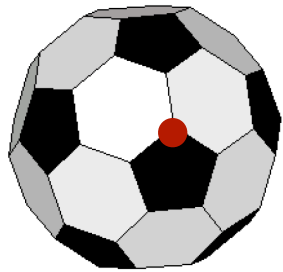
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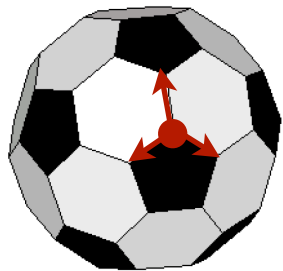
Representation conversion problem

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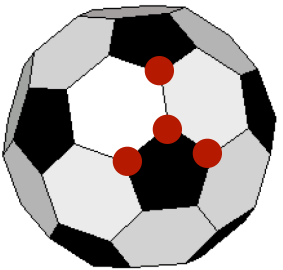
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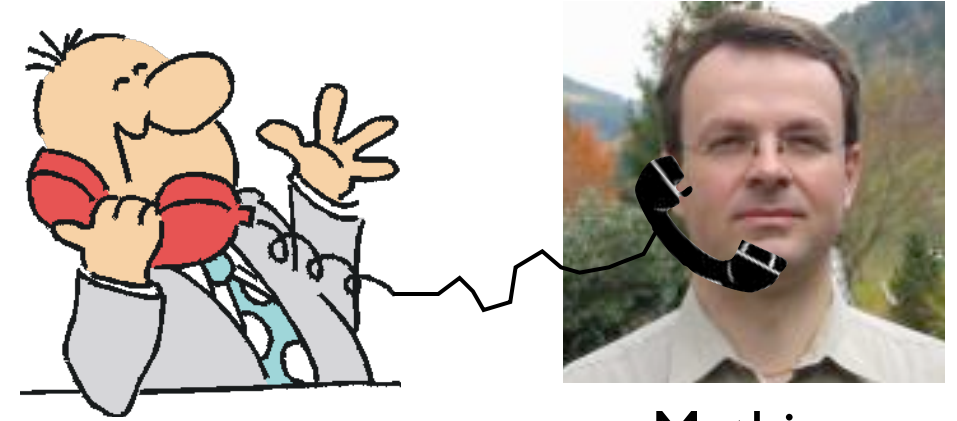
**BOTTLENECK:** Stabilizer and In-Orbit computations

=> Need of efficient data structures and algorithms for permutation groups: BSGS, (partition) backtracking

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Best known Algorithm:



Mathieu

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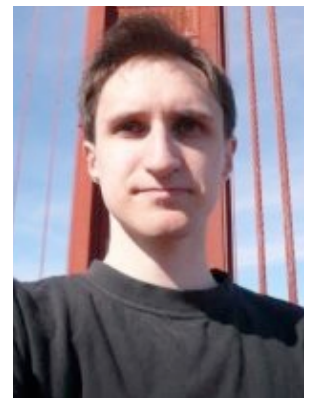
Mathieu

A C++-Tool



also available through **polymake** 

- helps to compute linear automorphism groups
- converts polyhedral representations using



Thomas Rehn  
(Phd 2014)

Recursive Decomposition Methods (Incidence/Adjacency)

# Applicaton: Lattice Sphere Packings

The **lattice sphere packing problem** can be phrased as:

Minimize  $(\det Q)^{1/n}$  on

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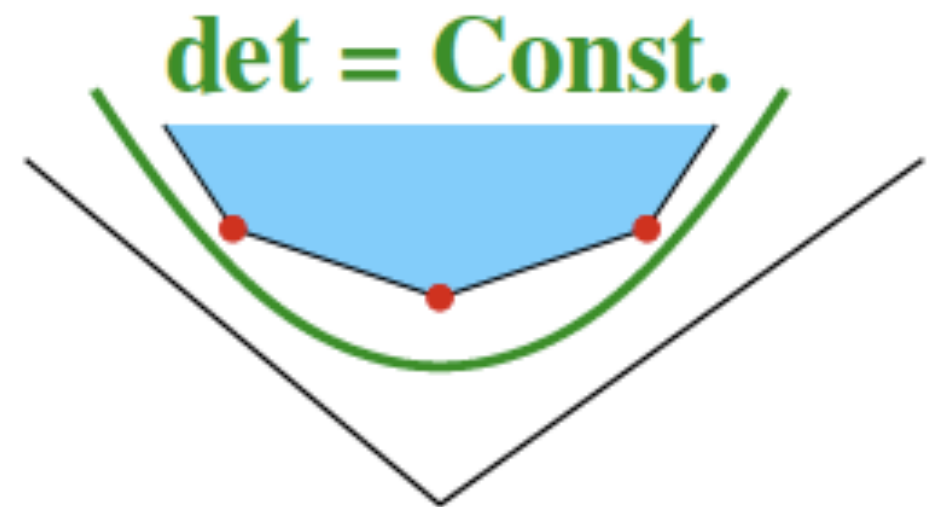
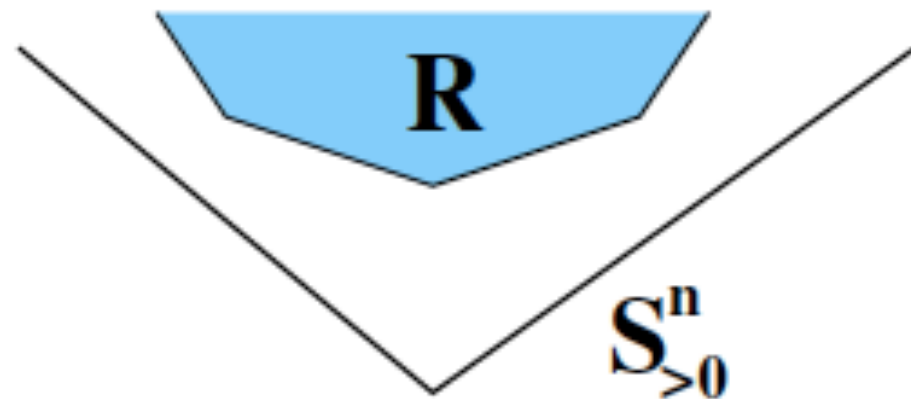


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$\min_{Q \in \mathcal{R}} (\det Q)^{1/n}$  is attained at vertices of  $\mathcal{R}$  (**perfect forms**)

Part II:

Koecher's generalization  
and T-perfect forms

# Koecher's generalization

1960/61 Max Koecher generalized  
Voronoi's reduction theory and proofs  
to a **setting with a self-dual cone  $C$**



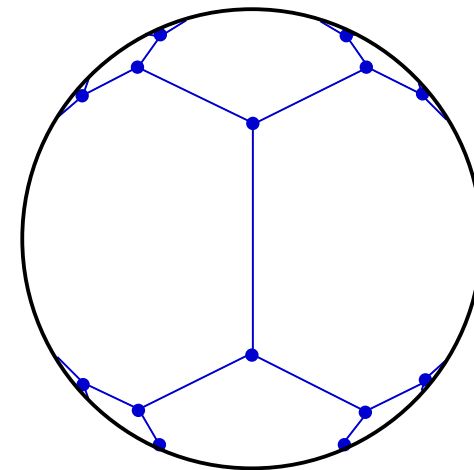
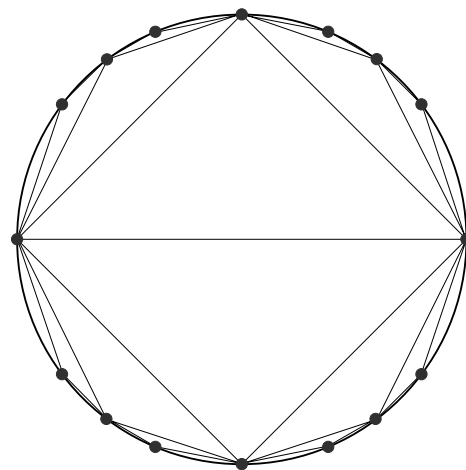
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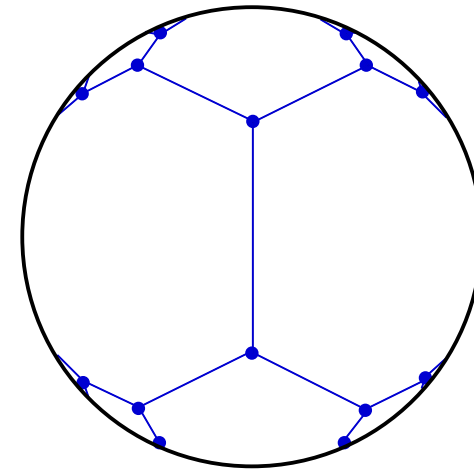
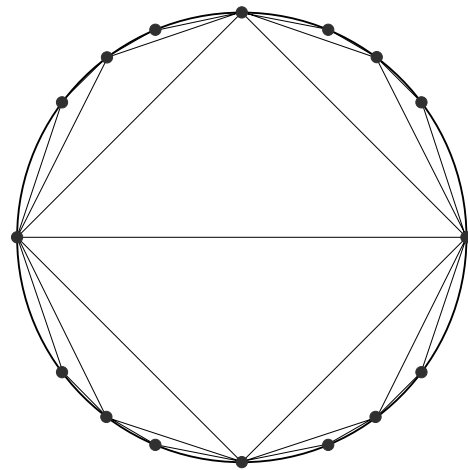
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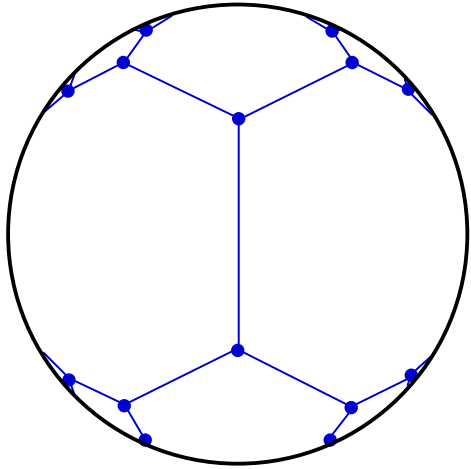


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Can in particular be applied to obtain reduction domains  
for the action of  $GL_n(\mathcal{O}_K)$  on suitable quadratic spaces

# Applications in Math

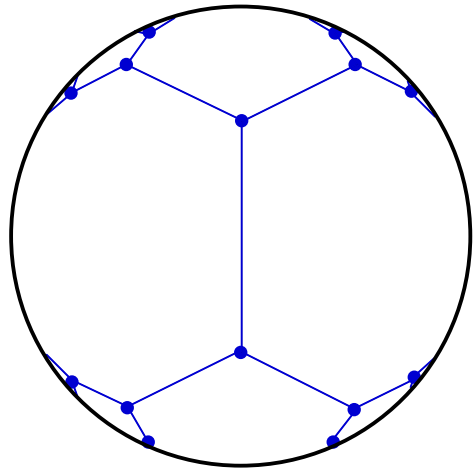
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Representation  
Conversion

Vertices / Perfect Forms:

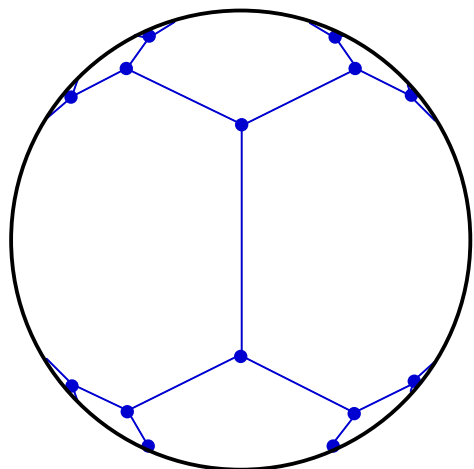
- Reduction theory
- Hermite constant

Polyhedral complex:

- Cohomology of  $GL_n(\mathcal{O}_K)$
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- Compactifications of moduli spaces of Abelian varieties

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## Ryshkov Polyhedron



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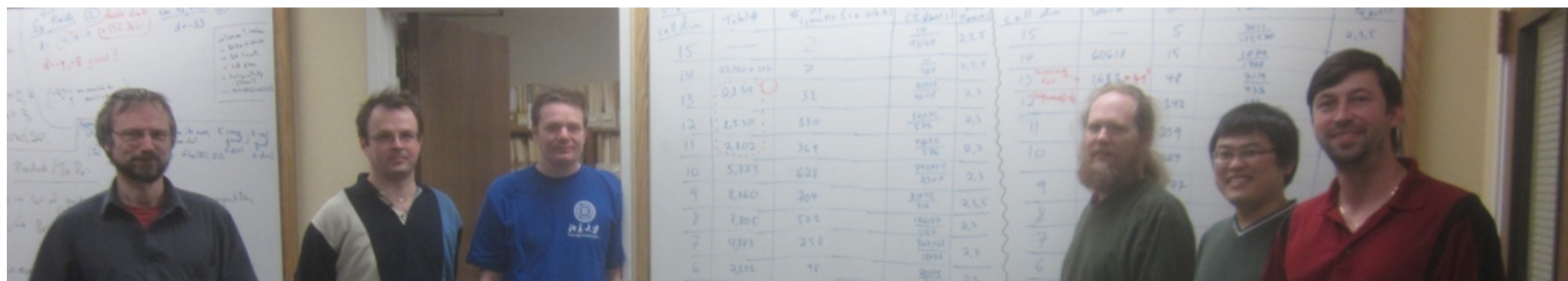
See Mathieu's talk  
after the coffee break!

Vertices / Perfect Forms:

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AIM Square group 2012: Gangl, Dutour Sikirić, Schürmann, Gunnells, Yasaki, Hanke



# Embedding Koecher's theory

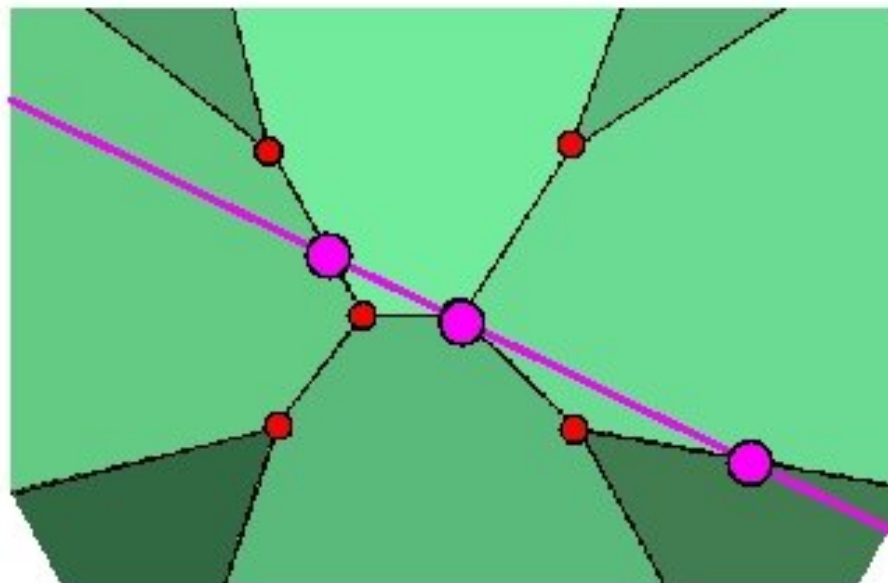
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Intersect Ryshkov polyhedron  $\mathcal{R}$  with a linear subspace  $T \subset \mathcal{S}^n$

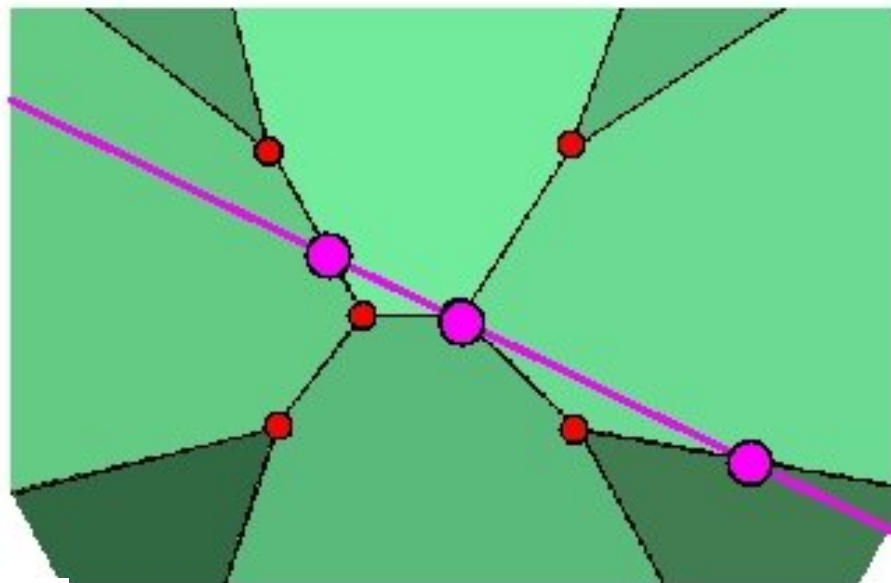


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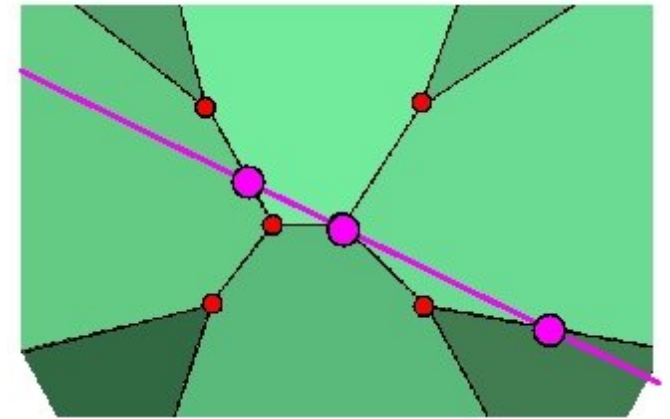
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**DEF:**  $Q \in T \cap \mathcal{S}_{>0}^n$  is  **$T$ -perfect** if it is a vertex of  $\mathcal{R} \cap T$

# Voronoi's Algorithm

for a linear subspace  $T$



SVPs: Obtain a  $T$ -perfect form  $Q$

1. SVP: Compute  $\text{Min } Q$  and describing inequalities of the polyhedral cone

$$\mathcal{P}(Q) = \{ Q' \in T : Q'[x] \geq 1 \text{ for all } x \in \text{Min } Q \}$$

2. PolyRepConv: Enumerate extreme rays  $R_1, \dots, R_k$  of  $\mathcal{P}(Q)$

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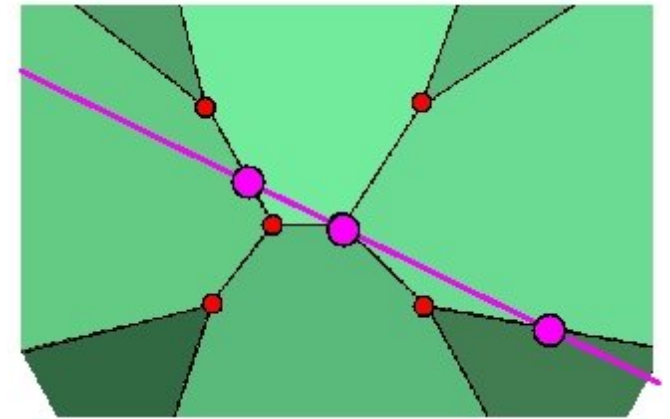
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Possible  
existence of  
“Dead-Ends”  
(for PQFs  $R$ )

# G-invariant theory

$Q, Q' \in T \cap \mathcal{S}_{>0}^n$  are called  **$T$ -equivalent**, if  $\exists U \in \mathrm{GL}_n(\mathbb{Z})$  with

$$Q' = U^t Q U \quad \text{and} \quad T = U^t T U$$

For a finite group  $G \subset \mathrm{GL}_n(\mathbb{Z})$  the **space of invariant forms**

$$T_G := \{ Q \in \mathcal{S}^n : G \subset \mathrm{Aut} Q \}$$

is a linear subspace of  $\mathcal{S}^n$ ;  $T_G \cap \mathcal{S}_{>0}^n$  is called **Bravais space**

**THM (Jaquet-Chiffelle, 1995):**

$$\{ T_G\text{-perfect } Q : \lambda(Q) = 1 \} / \sim_{T_G} \text{ finite}$$

# Applicaton: Lattice Sphere Packings

with prescribed symmetry

$n$	2	4	6	8	10	12
# $\mathcal{E}$ -perfect	1	1	2	5	1628	?
maximum $\delta$	0.9069...	0.6168...	0.3729...	0.2536...	0.0360...	

**Perfect Eisenstein forms**

$n$	2	4	6	8	10	12
# $\mathcal{G}$ -perfect	1	1	1	2	$\geq 8192$	?
maximum $\delta$	0.7853...	0.6168...	0.3229...	0.2536...		

**Perfect Gaussian forms**

$n$	4	8	12	16
# $\mathcal{Q}$ -perfect	1	1	8	?
maximum $\delta$	0.6168...	0.2536...	0.03125...	

**Perfect Quaternion forms**

PART III:

A new Generalization



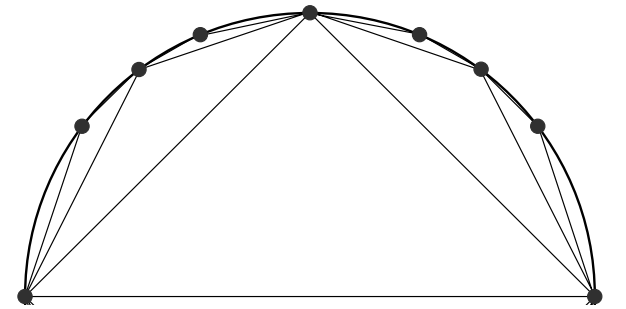
# Further Generalization? ... and application!

IDEA: Generalize Voronoi's theory to  
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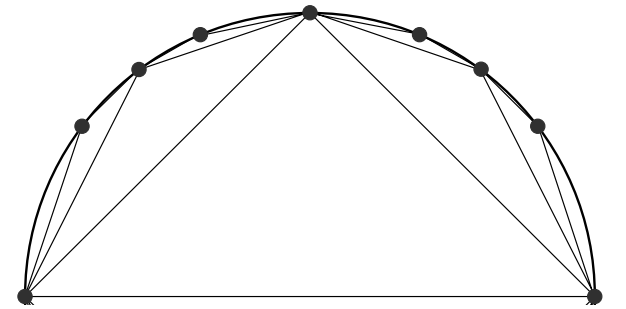
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In particular to the **completely positive cone**



# Further Generalization? ... and application!

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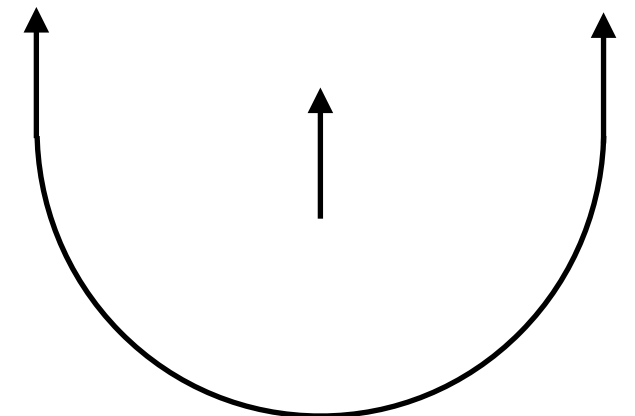


In particular to the **completely positive cone**

$\mathcal{CP}_n = \text{cone}\{xx^\top : x \in \mathbb{R}_{\geq 0}^n\}$  and its dual, the **copositive cone**

$$\begin{aligned}\mathcal{COP}_n &= (\mathcal{CP}_n)^* = \{B \in \mathcal{S}^n : \langle A, B \rangle \geq 0 \text{ for all } A \in \mathcal{CP}_n\} \\ &= \{B \in \mathcal{S}^n : B[x] \geq 0 \text{ for all } x \in \mathbb{R}_{\geq 0}^n\}\end{aligned}$$

$$\mathcal{CP}_n \subset \mathcal{S}_{>0}^n \subset \mathcal{COP}_n$$



$\langle A, B \rangle = \text{Trace}(A \cdot B)$  denotes the standard inner product on  $\mathcal{S}^n$

# Application: Copositive Optimization

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- Copositive optimization problems are **convex conic problems**

$$\begin{aligned} \min \langle C, Q \rangle \quad & \text{such that } \langle Q, A_i \rangle = b_i, \quad i = 1, \dots, m \\ & \text{and } Q \in \text{CONE} \end{aligned}$$

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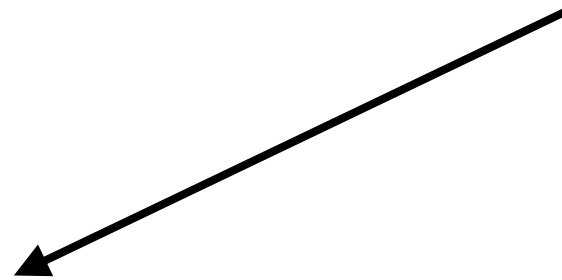
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**NP-hard (2000)**

Such problems have a duality theory and allow certificates for solutions!

# cp-factorizations and certificates

**DEF:** A finite set  $X \subset \mathbb{R}_{\geq 0}^n$  is called a **certificate**  
for  $Q \in \mathcal{S}^n$  being completely positive,  
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Known approaches so far:

- Anstreicher, Burer and Dickinson (in Dickinson's thesis 2013)  
give an **algorithm only for matrices in interior** based on ellipsoid method
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None of these approaches is exact and latter do not even guarantee to find solutions!

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(COP-SVP)

**DEF:**  $\min_{\text{COP}} Q = \min_{x \in \mathbb{Z}_{\geq 0}^n \setminus \{0\}} Q[x]$  is the copositive minimum

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For  $Q \in \text{int } \mathcal{COP}_n$  we can construct a family of simplices  $\Delta^k$  in the standard simplex  $\Delta = \{x \in \mathbb{R}_{\geq 0}^n : x_1 + \dots + x_n = 1\}$  such that each  $\Delta^k$  has vertices  $v_1, \dots, v_n$  with  $v_i^\top Q v_j > 0$

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Computation in practice:

”**Fincke-Pohst strategy**” to compute  $\min_{\text{COP}} Q$  in each cone  $\Delta^k$

# Generalized Ryshkov polyhedron

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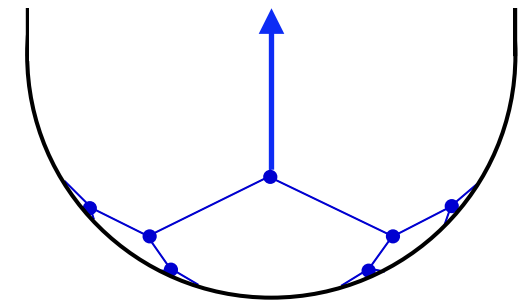
The set of all copositive quadratic forms / matrices  
with copositive minimum at least  $l$  is called  
**Ryshkov polyhedron**

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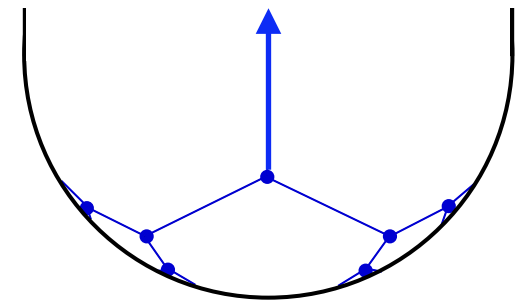


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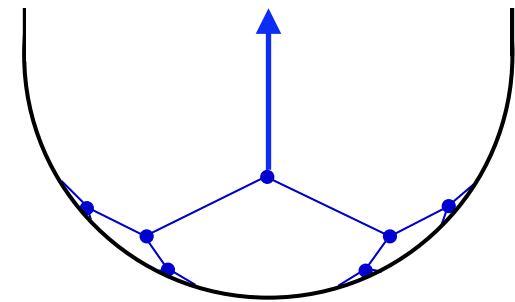
$Q$  is uniquely determined by  $\min_{\mathcal{COP}} Q$  and

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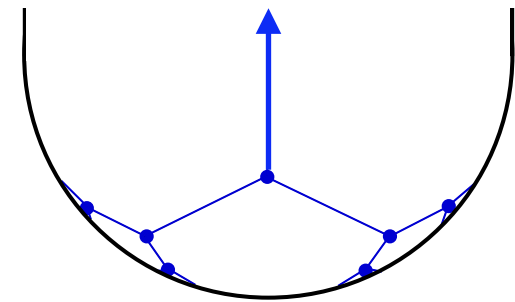
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2. **LP:** if  $A \in \text{cone} \{xx^\top : x \in \text{Min}_{\mathcal{COP}} B_P\}$  then **output**  $A \in \tilde{\mathcal{CP}}_n$
3. **COP-SVP:** Compute  $\text{Min}_{\mathcal{COP}} B_P$  and the polyhedral cone

$$\mathcal{P}(B_P) = \{ B \in \mathcal{S}^n : B[x] \geq 1 \text{ for all } x \in \text{Min}_{\mathcal{COP}} B_P \}$$

4. **PolyRepConv:** Determine a generator  $R$  of an extreme ray of  $\mathcal{P}(B_P)$  with  $\langle A, R \rangle < 0$ .
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with  $\langle A, R \rangle < 0$ . (flexible "pivot-rule")
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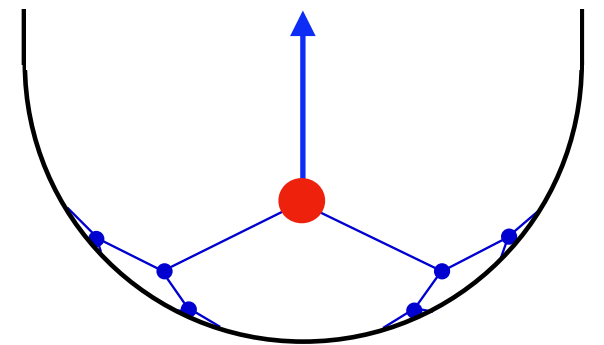
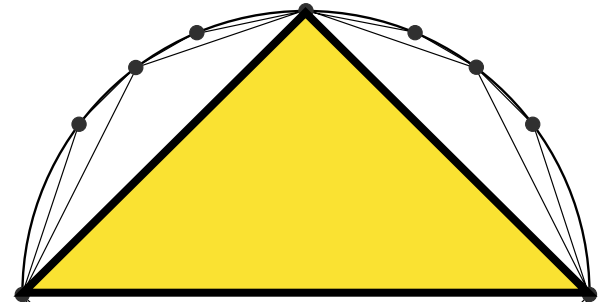
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# A copositive starting point

**THM:** 
$$\begin{pmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \dots & 0 & -1 & 2 \end{pmatrix}$$
 is  $\mathcal{COP}$ -perfect

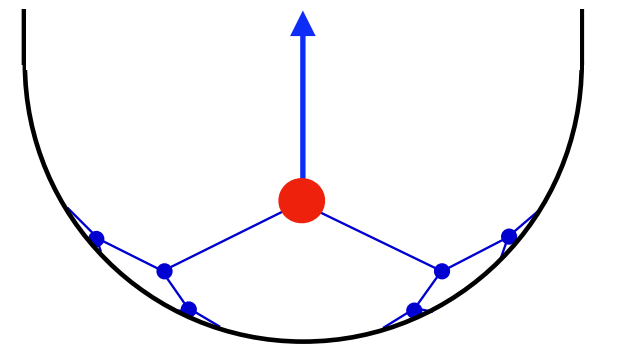
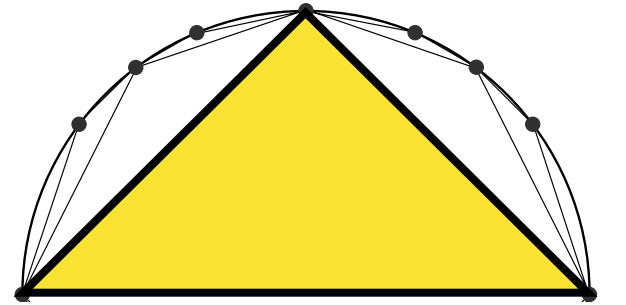
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*Proof.* Matrix  $Q_{A_n}$  is positive definite since

$$Q_{A_n}[x] = x_1^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2 \quad \text{for } x \in \mathbb{R}.$$

In particular it lies in the interior of the copositive cone. Furthermore,

$$\min_{\mathcal{COP}} Q_{A_n} = 2 \quad \text{with} \quad \text{Min}_{\mathcal{COP}} Q_{A_n} = \left\{ \sum_{i=j}^k e_j : 1 \leq j \leq k \leq n \right\}$$



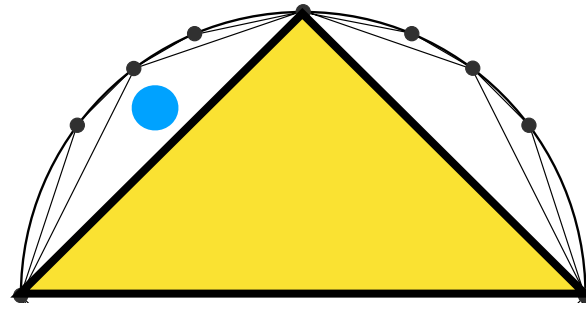
# Interior cases

(algorithm terminates)

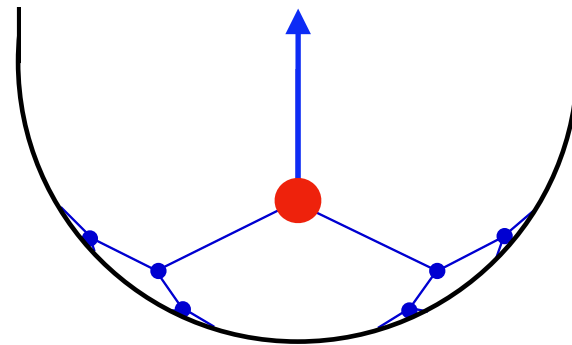
**EX:**  $A = \begin{pmatrix} 6 & 3 \\ 3 & 2 \end{pmatrix}$

# Interior cases

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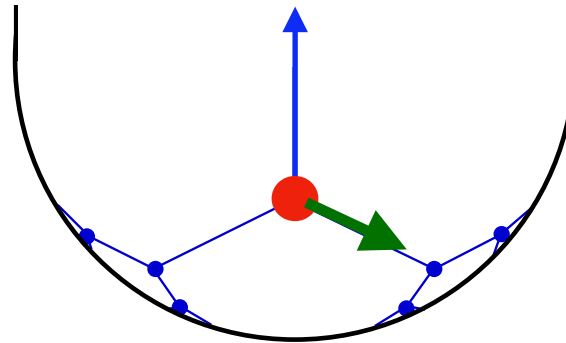
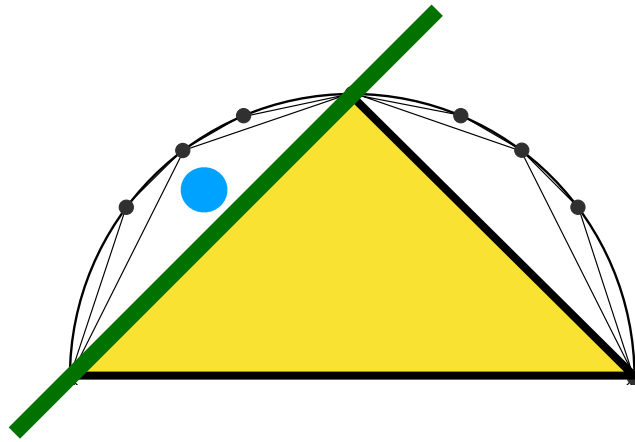
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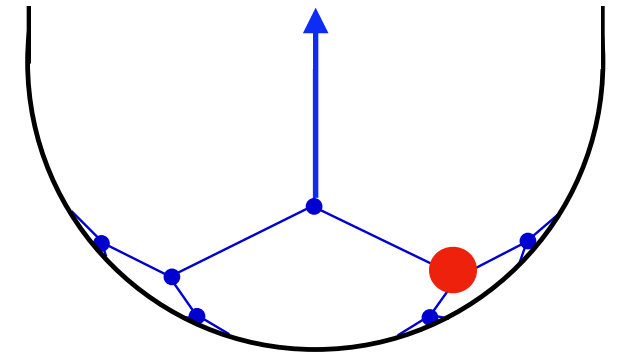
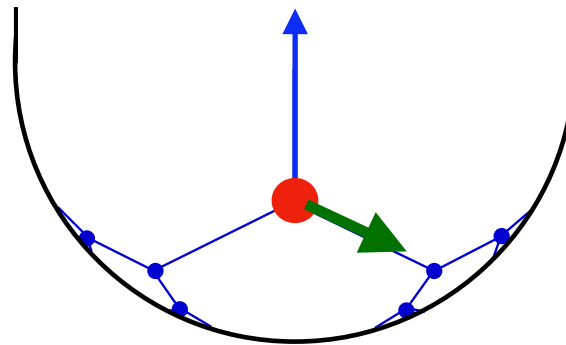
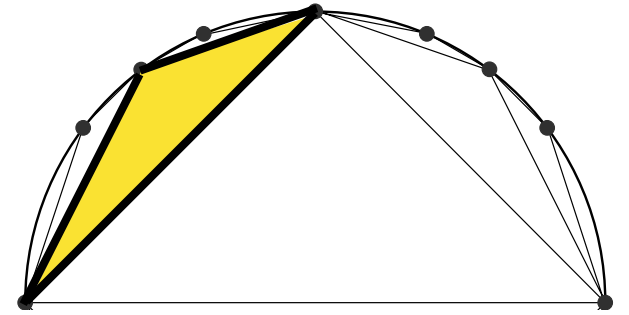
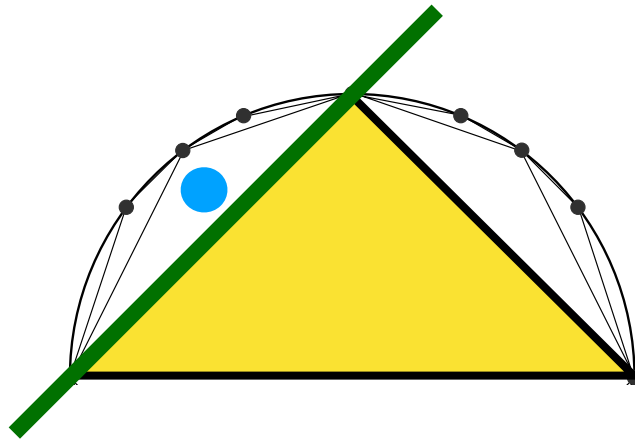
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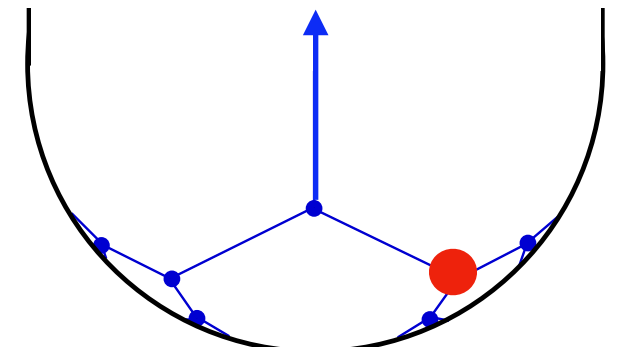
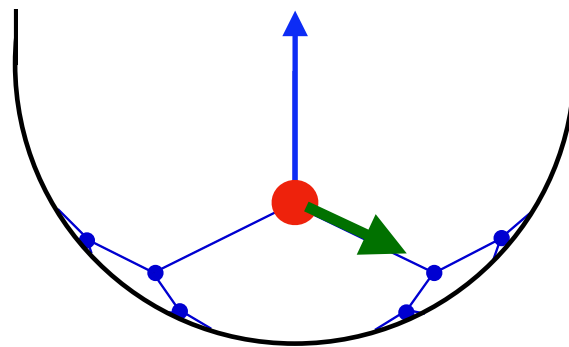
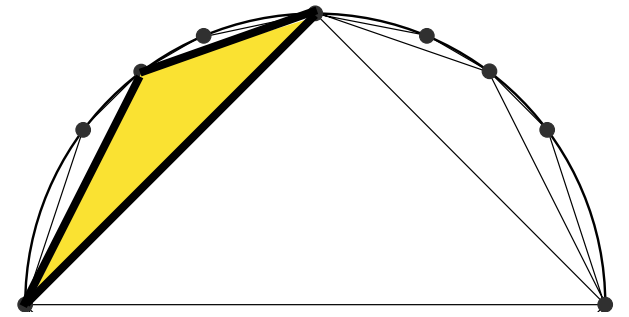
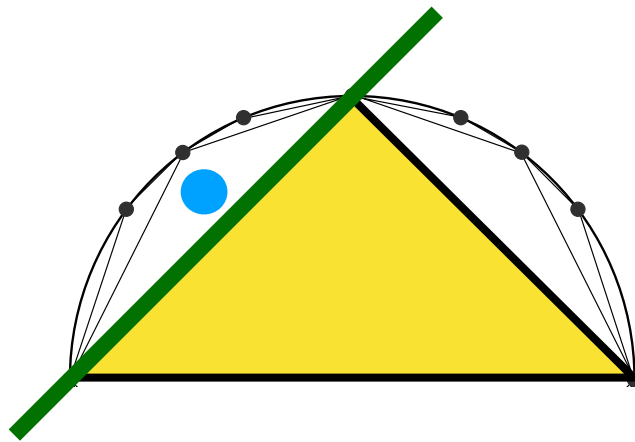
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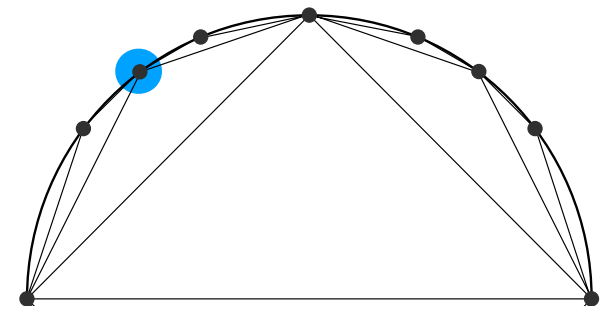
Starting with  $Q_{A_2}$  one iteration of the algorithm finds

the  $\mathcal{COP}$ -perfect matrix  $B_P = \begin{pmatrix} 1 & -3/2 \\ -3/2 & 3 \end{pmatrix}$  and

$$A = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}^\top + \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}^\top + \begin{pmatrix} 2 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix}^\top$$

# Boundary cases from $\mathcal{CP}_n$

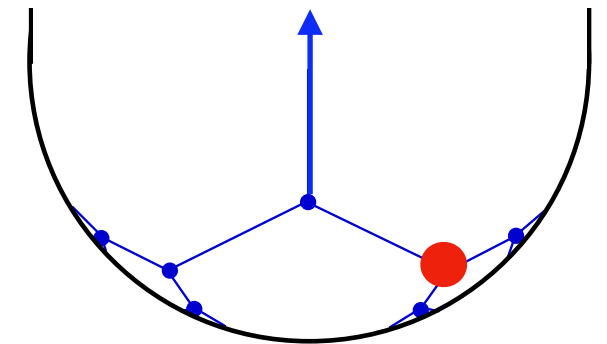
(algorithm terminates with a suitable pivot-rule)



**EX:**

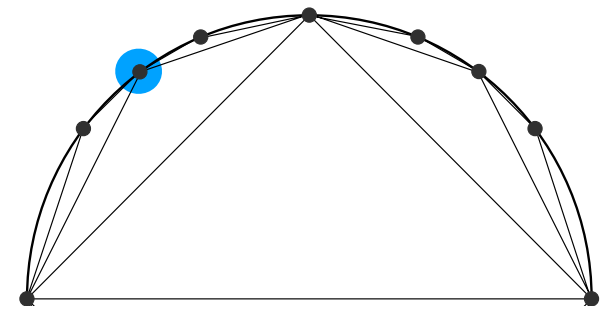
$$\begin{pmatrix} 8 & 5 & 1 & 1 & 5 \\ 5 & 8 & 5 & 1 & 1 \\ 1 & 5 & 8 & 5 & 1 \\ 1 & 1 & 5 & 8 & 5 \\ 5 & 1 & 1 & 5 & 8 \end{pmatrix}$$

from Groetzner, Dür (2018)  
not solved by their algorithms



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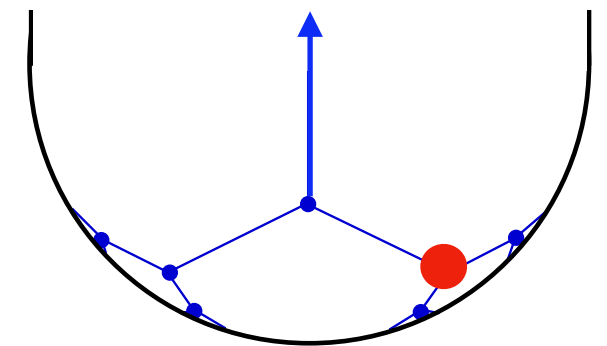
(algorithm terminates with a suitable pivot-rule)



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from Groetzner, Dür (2018)  
not solved by their algorithms



Starting with  $Q_{A_5}$ , our algorithm finds a cp-factorization after 5 iterations

$$v_1 = (0, 0, 0, 1, 1)$$

$$v_6 = (1, 0, 0, 0, 1)$$

$$v_2 = (0, 0, 1, 1, 0)$$

$$v_7 = (1, 0, 0, 1, 2)$$

$$v_3 = (0, 0, 1, 2, 1)$$

$$v_8 = (1, 1, 0, 0, 0)$$

$$v_4 = (0, 1, 1, 0, 0)$$

$$v_9 = (1, 2, 1, 0, 0)$$

$$v_5 = (0, 1, 2, 1, 0)$$

$$v_{10} = (2, 1, 0, 0, 1)$$

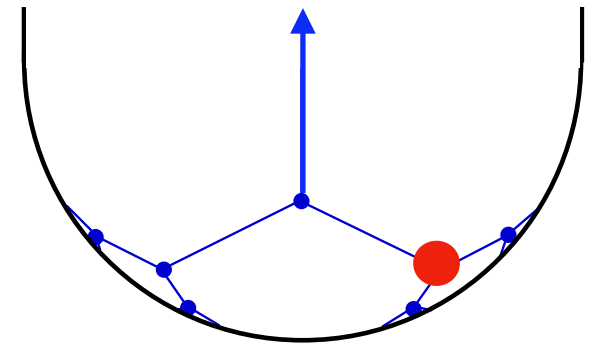
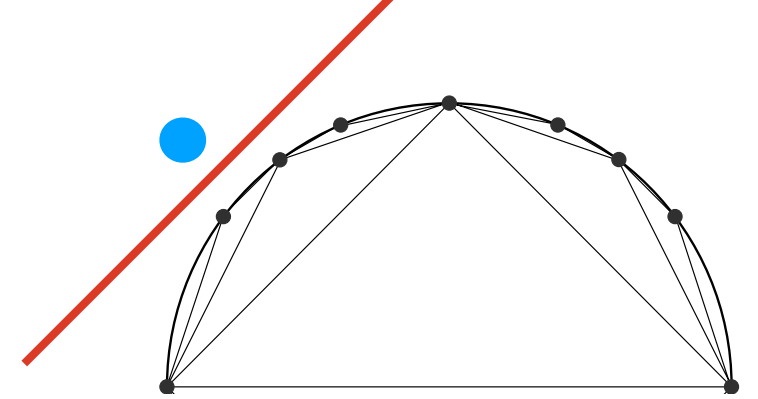
giving a **certificate for the matrix to be completely positive**

# Exterior cases

(algorithm conjectured to terminate)

**EX:** 
$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 1 & 6 \end{pmatrix}$$

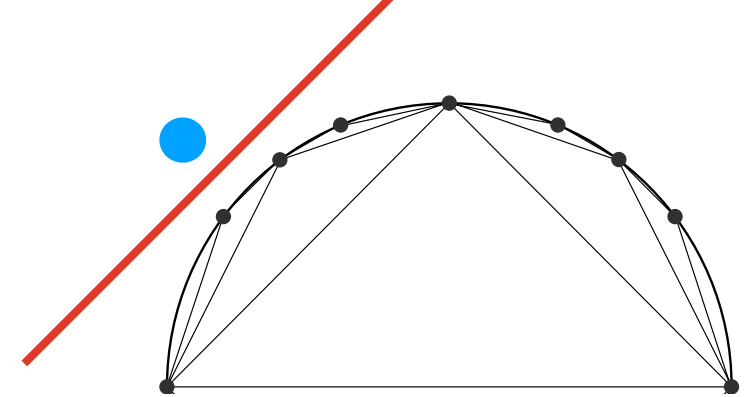
from Nie (2014)



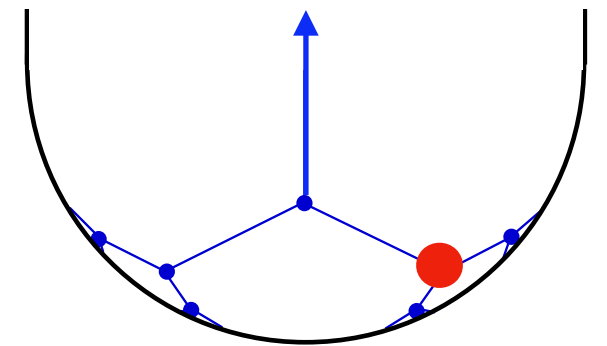


# Exterior cases

(algorithm conjectured to terminate)



**EX:** 
$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 1 & 6 \end{pmatrix}$$
 from Nie (2014)



Starting with  $Q_{A_5}$ , after 18 iterations our algorithm finds the  $\mathcal{COP}$ -perfect

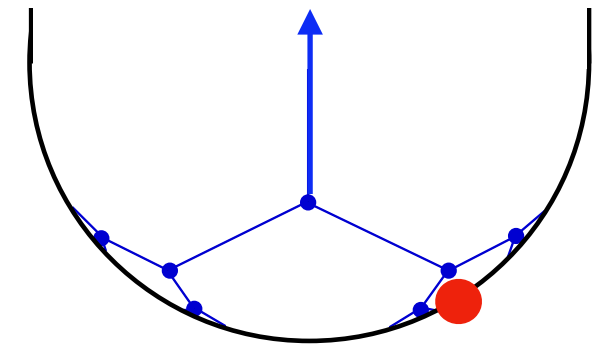
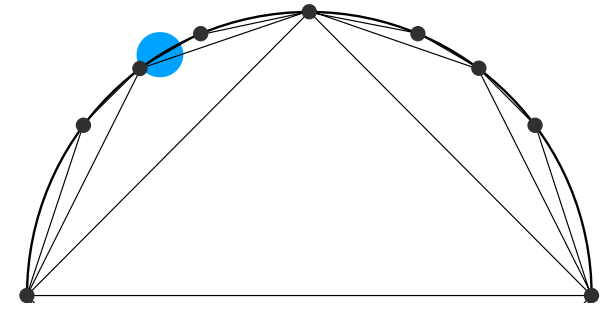
$$\begin{pmatrix} 363/5 & -2126/35 & 2879/70 & 608/21 & -4519/210 \\ -2126/35 & 1787/35 & -347/10 & 1025/42 & 253/14 \\ 2879/70 & -347/10 & 829/35 & -1748/105 & 371/30 \\ 608/21 & 1025/42 & -1748/105 & 1237/105 & -601/70 \\ -4519/210 & 253/14 & 371/30 & -601/70 & 671/105 \end{pmatrix}$$

giving a **certificate for the matrix not to be completely positive**

# Irrational boundary cases

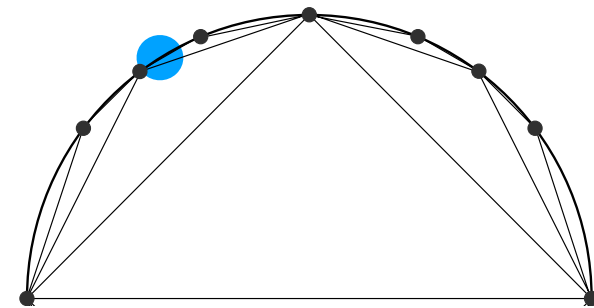
(algorithm is known not to terminate)

**EX:**  $A = \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix}^T = \begin{pmatrix} 2 & \sqrt{2} \\ \sqrt{2} & 1 \end{pmatrix}$

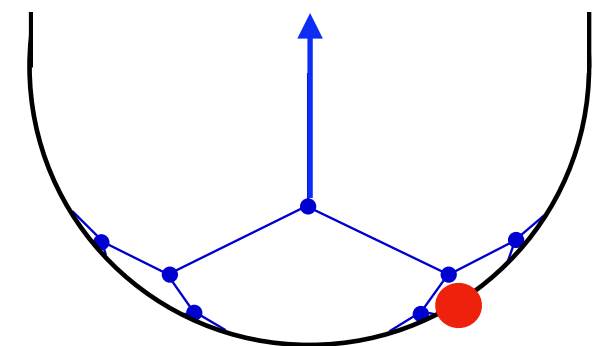


# Irrational boundary cases

(algorithm is known not to terminate)



**EX:**  $A = \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix}^\top = \begin{pmatrix} 2 & \sqrt{2} \\ \sqrt{2} & 1 \end{pmatrix}$



The  $\mathcal{CP}$ -perfect matrix after ten iterations of the algorithm is

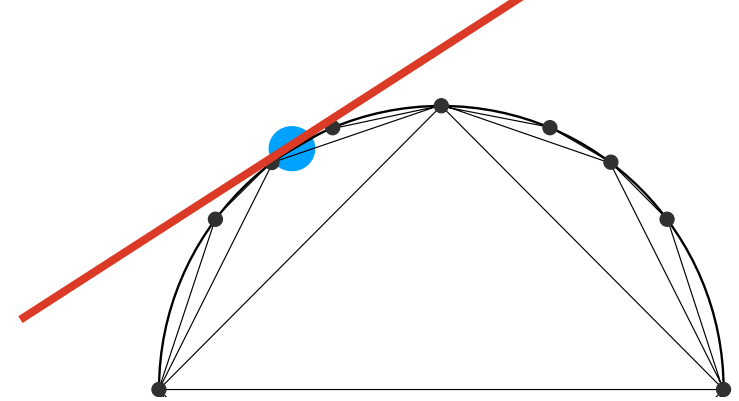
$$B_P^{(10)} = \begin{pmatrix} 4756 & -6726 \\ -6726 & 9512 \end{pmatrix}.$$

It can be shown that the matrices  $B_P^{(i)}$  converge to a multiple of

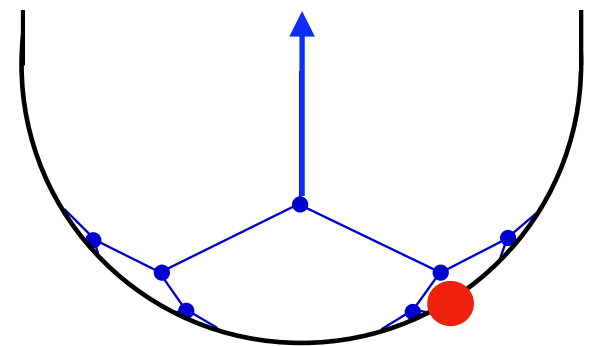
$$B = \begin{pmatrix} 1 & -\sqrt{2} \\ -\sqrt{2} & 2 \end{pmatrix} \text{ satisfying } \langle A, B \rangle = 0 \text{ and } \langle X, B \rangle \geq 0 \text{ for all } X \in \mathcal{CP}_2.$$

# Irrational boundary cases

(algorithm is known not to terminate)



**EX:** 
$$A = \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix}^\top = \begin{pmatrix} 2 & \sqrt{2} \\ \sqrt{2} & 1 \end{pmatrix}$$



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# References

- Mathieu Dutour Sikirić, Achill Schürmann and Frank Vallentin, Classification of eight dimensional perfect forms, *Electron. Res. Announc. Amer. Math. Soc.*, 13 (2007).
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