# Characterization of Logarithmic Fekete Critical Configurations of at Most Six Points in All Dimensions

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#### Outline

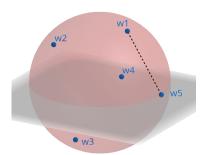
- Introduction
- Pormulation of Critical Configurations
- Five points
- 4 Six points
- **5** Conclusions and Future Work

#### Fekete Problem

Position n points on the sphere  $S^d \subset \mathbb{R}^{d+1}$ , so as to maximize the product of the distances between pairs of points:

$$\prod_{1 \le i < j \le n} ||w_i - w_j||,$$

$$w_i \in S^d \subset \mathbb{R}^{d+1}.$$

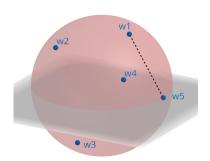


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Equivalently: place the points to minimize the logarithmic energy

$$E_{\log}(w) := -\sum_{1 \leq i < n} \log \left( \|w_i - w_j\|^2 \right), \quad w_i \in S^d \subset \mathbb{R}^{d+1}.$$

# Why caring about this problem?

Fekete problem: minimize the logarithmic energy on  $S^d$ :

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#### Smale's 7th problem for the next Century (1998) [4]

Give an "efficient" algorithm that, for each number of points n, finds  $\hat{w} \in (S^2)^n$  with optimal value up to a logarithmic factor:

$$E_{\log}(\hat{w}) - E_{\log}^* \le c \log(n)$$
, for a universal constant c.

## What is known about Fekete problem

- Optimal configurations known for few values of n and d.
- In  $S^2$ , optimals are known only for: n = 2, 3, 4, 5, 6 and 12.
- Optimal value known asymptotically, up to linear term [9]:

in 
$$S^2$$
:  $E_{\log}^* = \left(\frac{1}{2} - \log 2\right) \frac{n^2}{2} - \frac{n \log n}{4} + Cn + o(n), C =?$ 

- Any critical configuration satisfies:  $\sum_{i=1}^{n} w_i = \vec{0}$ .
- Has saddle-points [8, 10], and degenerate minima [11].
- Numerically: number of spurious local minima in  $S^2$  increases "dramatically" with n [2]; although none is known in  $S^2$ .
- Only one spurious local minima is known [8, 10]: n = 6 in  $S^3$ .



## Contributions and Approach

#### Contributions

- Formulate critical confs. as solutions of a polynomial system.
- Formulation is useful for any sphere  $S^d$ .
- For  $n \le 6$  points, and all sphere dimensions d, we:
  - recover previously known results in a Unified Framework.
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#### Approach

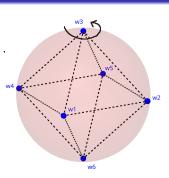
- Determine the number of exact solutions *m* of the formulation.
- $\bullet$  Find as many solutions as possible, until we reach m.

## Removing Orthogonal Symmetry

$$E_{\log}(w) := -\sum_{1 \le i < j \le n} \log (\|w_i - w_j\|^2).$$

Energy is invariant under rotations of the sphere.

This gives  $\infty$  solutions (but we need to count solutions).

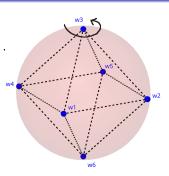


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#### Change of variables

Instead of the  $w_i$ , use dot products ("angles") as variables:

$$x_{ij} := w_i^T w_j = \cos(\theta_{ij}).$$

Rotations of a solution give the exact same solution (in the  $x_{ii}$ ).

Lagrange optimality conditions, expressed in the  $x_{ij} := w_i^T w_j$ :

$$(n-1)x_{ki} - \sum_{j=1, j\neq i}^{n} \frac{x_{ki} - x_{kj}}{1 - x_{ij}} = 0, \ \forall \ i \neq k.$$

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 (2)

Gives a polynomial expression, and ensures  $x_{ij} \neq 1$  ( $w_i \neq w_j$ ).

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Variables:  $x_{ij}$ ,  $z_{ij}$ , i < j.

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Variables:  $x_{ij}$ ,  $z_{ij}$ , i < j.

#### Number of variables and equations

	n	3	4	5	6	7	8
variables	$2\binom{n}{2}$	6	12	20	30	42	56
equations	n(3n-1)/2	12	22	35	51	70	92

## Number of solutions for n = 5 points (any sphere)

#### Gröbner theory

- Let I be the ideal generated by the polynomials of the system.
- Given a Gröbner basis of *I*, its Leading Monomials determine:
  - $\bigcirc$  if the system has a finite number of solutions: dim(I) = 0, and
  - 2 in that case, the exact number of solutions: deg(I).
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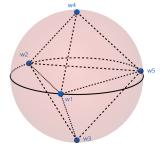
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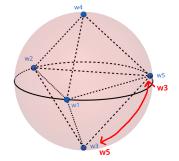
#### Next step

Search for solutions, until we match the 38 existent.

Easy to check that a particular critical conf. for n = 5 in  $S^2$  is 1:3:1.

Some permutations give different solutions in  $x_{ij}$ , but of same "kind".

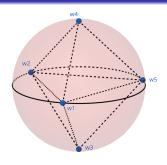


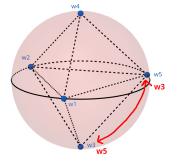




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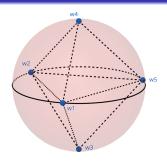


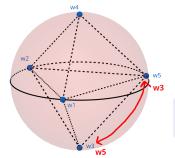


Given a "kind" of solution: how many permutations of the points  $w_i$  give different solutions in the variables  $x_{ij}$ ?

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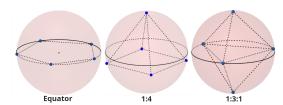


Given a "kind" of solution: how many permutations of the points  $w_i$  give different solutions in the variables  $x_{ii}$ ?

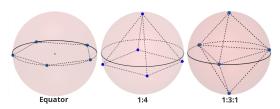
We find this number by trying all possible n! permutations.



We can easily imagine other kind of solutions.



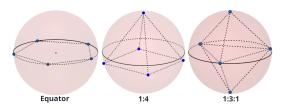
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The different permutations of each kind are:

Conf.	Equator	1:4	1:3:1	4-simplex	Found	Existent
$\neq$ perms.	12	15	10	1	38	38
sphere	$S^1$		$S^2$	<i>S</i> <sup>3</sup>		

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#### Theorem (For n = 5 points)

The only kind of critical configurations are the ones we imagined.

## Number of solutions for n = 6 (any sphere)

We find a Gröbner base with GRevLex monomial order (*msolve*), and then use it to determine the number of solutions (*Macaulay2*).

n	dim /	deg I
6	0	938

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## Possible values of dot product for n = 6

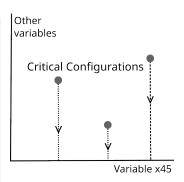
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# Approach to determine all the solutions

- Project solution set onto variable x<sub>45</sub>.
- Gives possible values of  $x_{45}$ .
- Finding a Gröbner base of the ideal, with elimination order that eliminates all variables except x<sub>45</sub>.



## Possible values of dot product for n = 6

#### Projected ideal is a PID:

$$I \cap \mathbb{Q}[x_{45}] = (p)$$
, some  $p$ .

Roots of generator p are the possible values of  $x_{45}$ .

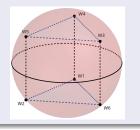
Generator Factor	Roots
x <sub>45</sub>	0
$(x_{45}+1)^2$	-1
$2x_{45}-1$	1/2
$2x_{45} + 1$	-1/2
$(5x_{45}-1)^2$	1/5
$5x_{45} + 1$	-1/5
$(5x_{45}+7)^2$	-7/5
$(5x_{45}^2 + 1)^2$	$\pm \frac{i}{\sqrt{5}}$
$5x_{45}^2 - 22x_{45} + 5$	$\frac{11\pm4\sqrt{6}}{5}$
$5x_{45}^2 + 2x_{45} - 1$	$\frac{-1\pm\sqrt{6}}{5}$
$5x_{45}^2 + 14x_{45} - 1$	$\frac{-7\pm3\sqrt{6}}{5}$
$25x_{45}^2 + 28x_{45} + 19$	$\frac{-14\pm i3\sqrt{31}}{25}$
$125x_{45}^2 + 50x_{45} - 31$ $100x_{45}^4 + 95x_{45}^4 - 21x_{45}^2 - 22x_{45} + 10$ $250x_{45}^4 + 110x_{45}^3 - 21x_{45}^2 - 19x_{45} + 4$	$\frac{-5\pm6\sqrt{5}}{25}$
$100x_{45}^4 + 95x_{45}^{35} - 21x_{45}^2 - 22x_{45} + 10$	4 complex
$250x_{45}^{4} + 110x_{45}^{3} - 21x_{45}^{2} - 19x_{45} + 4$	4 complex
$400x_{45}^4 + 488x_{45}^3 - 111x_{45}^{21} - 196x_{45} + 67$	4 complex
$3x_{45} + 1$	-1/3
$5x_{45} + 4$	-4/5
$10x_{45} - 1$	1/10
$25x_{45}-1$	1/25
$25x_{45} + 11$	-11/25
$25x_{45} + 23$	-23/25
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## Solutions for each coordinate value of $x_{45}$

# For each factor $p_i$ of the generator (each $x_{45}$ value)

- Add  $p_i = 0$  to the original system.
- Find solutions of simplified system, and count permutations.

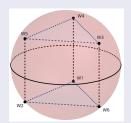


Configuration	# perms	Sphere
Equator	60	$S^1$
1:5	72	<i>S</i> <sup>2</sup>
1:4:1	15	S <sup>2</sup>
3:3	60+60	S <sup>2</sup>
Complex 1	90	S <sup>2</sup>
Complex 2	360	<i>S</i> <sup>2</sup>
Real 1	15	<i>S</i> <sup>3</sup>
Real 2	45	<i>S</i> <sup>3</sup>
Real 3	60	<i>S</i> <sup>3</sup>
Real 4	10	<i>S</i> <sup>3</sup>
5-simplex	1	S <sup>4</sup>
Found	848	
Existent	938	
Difference	938 - 848 = 90	

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Complex 1 has multiplicity 2: +90.

# Classification of **real** critical configurations (n = 6)

Configuration	$S^1$	$S^2$	$S^3$	$S^4$
Equator	GM	S	S	S
1:5	-	S	S	S
1:4:1	-	GM	S	S
$3:3(\sqrt{6})$	-	S	S	S
Real 1	-	-	SM	S
Real 2	-	-	S	S
Real 3	-	-	S	S
Real 4	-	-	GM	S
5-simplex	-	-	-	GM

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Real 2	-	-	S	S
Real 3	-	-	S	S
Real 4	-	-	GM	S
5-simplex	-	-	-	GM

- Global minima are classified comparing energy values.
- Other configurations classified with Hessian of the Lagrangian.
- It is known that problem does not admit local/global maxima.



- Formulate critical configurations as polynomial system sols.
- Obtain all critical configurations, and in particular all optimal configurations, for  $n \le 6$ ,  $d \ge 1$ .
- Give first exhaustive list of critical configurations and classification for n = 6 in  $S^2$ .

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#### Pros and Cons of our Approach

- √ Unified framework (previous results are from different articles).
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#### Future Work

- prove optimal configuration for n = 7 (numerical candidate  $\exists$ )
- "simplify" the system of equations, exploiting symmetries.

## Gracias por su atención

#### Code and presentation

http://www.github.com/matiasvd



#### Acknowledgments

- Cluster.UY for the hardware infrastructure.
- ANII and CAP for PhD grants.
- msolve, Macaulay2 and SymPy developers for their great work

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# *msolve* executions (n = 6 points)

AVX512 instructions, 20 threads, Xeon-Gold 6138.

GRevLex monomial order (msolve 0.73) - With null CM equations

msolve GB in	reduced	I GB size	
total time RAM		# pols	# mons
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#### GRevLex without lifting GB to $\mathbb{Q}$ (msolve 0.90)

	msolve GB		reduced GB size	
Null Center of Mass equations	total time	RAM	# pols	# mons
Yes	485 s	3.35 GB	2473	2.133.497
No	433 s	3.36 GB	2473	2.133.497

# Configurations for n = 6 points in $S^3 \subset \mathbb{R}^4$

#### Optimal configuration: Real 4

Two equilateral triangles, each inscribed in a copy of  $S^1$  lying in orthogonal spaces.

#### The other configurations

- Real 1 (SM): analogous to 1:4:1 of  $S^2$ : it has the poles, and then the optimal configuration for 4 points in the equatorial sphere.
- Real 3 (S): analogous to 1:5 of  $S^2$ : it has a pole, and then the optimal configuration for 5 points in the corresponding sphere.
- Real 2 (S): no analogous on  $S^2$ . Has 4 points on the Equator of a sphere and the optimal configuration for 2 points in another sphere. Line through these two points is orthogonal to the plane of the 4 point Equator.



## From $x_{ij}$ to $w_i$

Any solution in the variables  $w_i$  has an associated solution  $x_{ij} = w_i^T w_j$ . Reciprocal is also true in  $\mathbb{C}$ .

#### Theorem (Autonne-Takagi factorization [7, Corollary 2.6.6])

If  $X \in \mathbb{C}^{n \times n}$  is symmetric, there is a unitary  $P \in \mathbb{C}^{n \times n}$ , and a non-negative diagonal matrix  $D \in \mathbb{R}^{n \times n}$ , such that:  $X = P^T DP$ . Furthermore, the entries of D are the singular values of X.

#### Corollary

If  $X \in \mathbb{C}^{n \times n}$  is symmetric with rank d, and ones on its diagonal, there exists  $W \in \mathbb{C}^{d \times n}$ , such that:  $X = W^T W$ ,  $w_i^T w_i = 1$ ,  $\forall i$ .

#### Proof.

As X is symmetric:  $X = P^T DP$ . Take:  $W = \sqrt{\hat{D}P}$ ; where  $\hat{D} \in \mathbb{R}^{d \times n}$  is the submatrix of D with positive singular values.

