# Energy minimization via moment hierarchies

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As an optimization problem:

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- ► Hierarchy for packing problems [L.-Vallentin 2014]

 Hierarchy obtained by generalizing Lasserre's hierarchy from combinatorial optimization to the continuous setting

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 Towards computations using several types of symmetry reduction









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Theorem (Finite convergence) We have  $E_1 \leq \cdots \leq E_N = E$ 

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- The dual program:

$$E_t^* = \sup\left\{\sum_{i=0}^s {N \choose i} a_i : a_0, \dots, a_s \in \mathbb{R}, \ K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K \le h \text{ on } I_{=i} \text{ for } i = 0, \dots, s\right\}$$

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#### Theorem

Strong duality holds: 
$$E_t = E_t^*$$
 for each t

# Closing the gaps



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▶ Define  $E_{t,d}^*$  by replacing the cone  $C(I_t \times I_t)_{\succeq 0}$  in  $E_t^*$  by a finite dimensional inner approximating cone  $C_d$ 

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- ▶ Let  $e_1, e_2, \ldots$  be a dense sequence in  $\mathcal{C}(I_t)$  and define

$$C_d = \big\{ \sum_{i,j=1}^d F_{i,j} e_i \otimes e_j : F \in \mathbb{R}^{d \times d} \text{ positive semidefinite} \big\}$$

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#### Theorem

If V is a compact metric space, then  $E^*_{t,d} \to E^*_t$  as  $d \to \infty$  for all t

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- ▶  $C(V)^{\odot t}$  can be written in terms of tensor products of the irreducible subspaces of C(V)
- ► If we know how to decompose C(V) into irreducibles, and how to decompose tensor products of those irreducibles into irreducibles, then we have a symmetry adapted basis of V<sub>t</sub>

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- ▶ Invariant theory: there is a polynomial q such that  $p(x_1, \ldots, x_4) = q(x_1 \cdot x_2, \ldots, x_3 \cdot x_4)$
- Model nonnegativity constraints as sum of squares constraints using Putinar's theorem from real algebraic geometry

- We know how to these decompositions from the quantum mechanics literature (angular momentum coupling): use Clebsch-Gordan coefficients
- ► The affine constraints in E<sup>\*</sup><sub>t,d</sub> are nonnegativity constraints of a polynomial p ∈ ℝ[x<sub>1</sub>,...,x<sub>4</sub>], where each x<sub>i</sub> is a vector of 3 variables (the coefficients of these polynomials depend on the entries in the block diagonalization of F)
- We have  $p(\gamma x_1, \ldots, \gamma x_4) = p(x_1, \ldots, x_4)$  for all  $\gamma \in O(3)$
- ▶ Invariant theory: there is a polynomial q such that  $p(x_1, \ldots, x_4) = q(x_1 \cdot x_2, \ldots, x_3 \cdot x_4)$
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- ► A sum of squares polynomial s can be written as s(x) = v(x)<sup>T</sup>Qv(x), where Q is a positive semidefinite matrix and v(x) a vector containing all monomials up to some degree

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- ► Using a reduction to 3 variables using trigonometric polynomials we compute that E<sub>2</sub> = E (up to solver precision)

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Thank you!