New bounds for spherical finite distance sets

David de Laat (ICERM/MIT) Fabrício Machado (Universidade de São Paulo) Fernando Oliveira (TU Delft) Frank Vallentin (Universität zu Köln)

Computation and Optimization of Energy, Packing, and Covering, 11 April 2018, ICERM



Example: the Petersen graph



Example: the Petersen graph



Example: the Petersen graph

- In general difficult to solve to optimality (NP-hard)



Example: the Petersen graph

- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number



Example: the Petersen graph

- In general difficult to solve to optimality (NP-hard)
- The Lovász ϑ -number upper bounds the independence number
- Can be computed through semidefinite programming (SDP)

Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Motivating example: The spherical cap packing problem

Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Motivating example: The spherical cap packing problem

- As vertex set we take the unit sphere

Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Motivating example: The spherical cap packing problem

- As vertex set we take the unit sphere
- Distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Motivating example: The spherical cap packing problem

- As vertex set we take the unit sphere
- Distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



- Optimal density given by the independence number $\alpha(G)$

Definition (L-Vallentin 2015)

A graph whose vertex set is a Hausdorff space is a *topological* packing graph if each finite clique is contained in an open clique

Motivating example: The spherical cap packing problem

- As vertex set we take the unit sphere
- Distinct vertices x and y are adjacent if the spherical caps centered about x and y intersect in their interiors:



- Optimal density given by the independence number lpha(G)
- [Bachoc-Nebe-Oliveira-Vallentin 2009] showed the Delsarte bound can be interpreted as the ϑ -number of this graph

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies
- Let I be the set of independent sets in the graph

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies
- Let I be the set of independent sets in the graph
- Consider graphs where the quotient I/Γ is finite

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies
- Let I be the set of independent sets in the graph
- Consider graphs where the quotient I/Γ is finite

Motivating example: Spherical finite distance graphs

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies
- Let I be the set of independent sets in the graph
- Consider graphs where the quotient I/Γ is finite

Motivating example: Spherical finite distance graphs

- Two vertices $x, y \in S^{n-1}$ are adjacent if $x \cdot y \not\in \{1, a_1, \dots, a_r\}$

- The symmetry group Γ of a topological packing graph G is the group of all autohomeomorphisms of the vertices preserving adjacencies and nonadjacencies
- Let I be the set of independent sets in the graph
- Consider graphs where the quotient I/Γ is finite

Motivating example: Spherical finite distance graphs

- Two vertices $x, y \in S^{n-1}$ are adjacent if $x \cdot y \not\in \{1, a_1, \dots, a_r\}$
- $|I/\Gamma|<\infty$ follows from the fact that any two isometric sets in \mathbb{R}^n are related by an isometry of \mathbb{R}^n

- Can use bounds for spherical finite distance graphs to obtain bounds on the maximum number of equiangular lines and nonexistence proofs of strongly regular graphs

- Can use bounds for spherical finite distance graphs to obtain bounds on the maximum number of equiangular lines and nonexistence proofs of strongly regular graphs
- The Delsarte 2-point bound and Bachoc-Vallentin 3-point bound have been studied extensively in the context of spherical finite distance graphs and equiangular lines [Delsarte, Goethals, Seidel, Barg, Yu, King, Tang, Glazyrin]

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$
- $\mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$ cone of continuous maps $T \colon V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$
- $\mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$ cone of continuous maps $T \colon V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

Definition (L-Machado-Oliveira-Vallentin 2018) $\Delta_k(G)^* = \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ B_kT \le (\alpha - 1)\mathbf{1}_{I=1} - 2\mathbf{1}_{I=2} \right\}$

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $C(V^2 \times I_{k-2})_{\geq 0}$ cone of continuous maps $T \colon V^2 \times I_{k-2} \to \mathbb{R}$
 - where each $(x,y)\mapsto T(x,y,Q)$ is a positive kernel

 $\begin{aligned} \text{Definition (L-Machado-Oliveira-Vallentin 2018)} \\ \Delta_k(G)^* &= \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ & B_k T \leq (\alpha - 1) \mathbf{1}_{I=1} - 2 \mathbf{1}_{I=2} \right\} \\ B_k \colon \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) &= \sum_{\substack{Q \subseteq S:\\ |Q| \leq k-2}} \sum_{\substack{x,y \in S:\\ \{x,y\} \cup Q = S}} T(x,y,Q) \end{aligned}$

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $\mathcal{C}(V^2 \times I_{k-2})_{\geq 0}$ cone of continuous maps $T: V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

 $\begin{aligned} & \mathsf{Definition} \ \ (\mathsf{L}\text{-Machado-Oliveira-Vallentin 2018}) \\ & \Delta_k(G)^* = \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ & B_k T \leq (\alpha - 1) \mathbf{1}_{I=1} - 2 \mathbf{1}_{I=2} \right\} \\ & B_k \colon \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) = \sum_{\substack{Q \subseteq S : \\ |Q| \leq k-2}} \sum_{\substack{x, y \in S : \\ \{x, y\} \cup Q = S}} T(x, y, Q) \end{aligned}$

- $\alpha(G) \leq \Delta_k(G)^*$ for all compact topological packing graphs G

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $\mathcal{C}(V^2 \times I_{k-2})_{\geq 0}$ cone of continuous maps $T: V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

Definition (L-Machado-Oliveira-Vallentin 2018) $\Delta_k(G)^* = \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ B_k T \leq (\alpha - 1)\mathbf{1}_{I_{=1}} - 2\mathbf{1}_{I_{=2}} \right\}$ $B_k : \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) = \sum_{\substack{Q \subseteq S: \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S: \\ \{x,y\} \cup Q = S}} T(x, y, Q)$

- $\alpha(G) \leq \Delta_k(G)^*$ for all compact topological packing graphs G
- $\Delta_2(G)$ is the Lovász ϑ -number (Delsarte bound)

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $\mathcal{C}(V^2 \times I_{k-2})_{\geq 0}$ cone of continuous maps $T: V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

 $\begin{array}{l} \text{Definition (L-Machado-Oliveira-Vallentin 2018)} \\ \Delta_k(G)^* &= \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ & B_k T \leq (\alpha - 1) \mathbf{1}_{I=1} - 2 \mathbf{1}_{I=2} \right\} \\ B_k \colon \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) &= \sum_{\substack{Q \subseteq S : \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S : \\ \{x,y\} \cup Q = S}} T(x,y,Q) \end{array}$

- $\alpha(G) \leq \Delta_k(G)^*$ for all compact topological packing graphs G
- $\Delta_2(G)$ is the Lovász artheta-number (Delsarte bound)
- $\Delta_3(G)$ is essentially the Bachoc-Vallentin 3-point bound

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $\mathcal{C}(V^2 \times I_{k-2})_{\geq 0}$ cone of continuous maps $T: V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

Definition (L-Machado-Oliveira-Vallentin 2018)
$$\begin{split} \Delta_k(G)^* &= \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}, \\ B_k T \leq (\alpha - 1) \mathbf{1}_{I=1} - 2\mathbf{1}_{I=2} \right\} \\ B_k \colon \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) = \sum_{\substack{Q \subseteq S : \\ |Q| \leq k-2}} \sum_{\substack{x, y \in S : \\ \{x, y\} \cup Q = S}} T(x, y, Q) \end{split}$$

- $\alpha(G) \leq \Delta_k(G)^*$ for all compact topological packing graphs G
- $\Delta_2(G)$ is the Lovász artheta-number (Delsarte bound)
- $\Delta_3(G)$ is essentially the Bachoc-Vallentin 3-point bound
- Stabilization at $\Delta_{\alpha(G)+2}(G),$ but no convergence proof

- I_{k-2} is the set of independent sets of cardinality $\leq k-2$ - $\mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}$ cone of continuous maps $T \colon V^2 \times I_{k-2} \to \mathbb{R}$ where each $(x, y) \mapsto T(x, y, Q)$ is a positive kernel

 $\begin{array}{l} \text{Definition (L-Machado-Oliveira-Vallentin 2018)} \\ \Delta_k(G)^* &= \inf \left\{ \alpha : \alpha \in \mathbb{R}, \ T \in \mathcal{C}(V^2 \times I_{k-2})_{\succeq 0}^{\Gamma}, \\ B_k T \leq (\alpha - 1) \mathbf{1}_{I=1} - 2 \mathbf{1}_{I=2} \right\} \\ B_k \colon \mathcal{C}(I_k \setminus \{\emptyset\}) \to \mathcal{C}(V^2 \times I_{k-2}), \ B_k T(S) = \sum_{\substack{Q \subseteq S : \\ |Q| \leq k-2}} \sum_{\substack{x,y \in S : \\ \{x,y\} \cup Q = S}} T(x,y,Q) \end{array}$

- $\alpha(G) \leq \Delta_k(G)^*$ for all compact topological packing graphs G
- $\Delta_2(G)$ is the Lovász ϑ -number (Delsarte bound)
- $\Delta_3(G)$ is essentially the Bachoc-Vallentin 3-point bound
- Stabilization at $\Delta_{\alpha(G)+2}(G),$ but no convergence proof
- $T(\gamma x,\gamma y,\gamma Q)=T(x,y,Q)$ for all $\gamma\in \Gamma$

Symmetry reduction

Lemma (L-Machado-Oliveira-Vallentin 2018) If I_{k-2}/Γ is finite, then we have the homeomorphism

$$\coprod_{R \in \mathcal{R}_{k-2}} V^2 / \mathrm{Stab}_{\Gamma}(R) \simeq (V^2 \times I_{k-2}) / \Gamma,$$

where \mathcal{R}_{k-2} a complete set of representatives of the orbits of I_{k-2}

Symmetry reduction

Lemma (L-Machado-Oliveira-Vallentin 2018) If I_{k-2}/Γ is finite, then we have the homeomorphism

$$\coprod_{R \in \mathcal{R}_{k-2}} V^2 / \mathrm{Stab}_{\Gamma}(R) \simeq (V^2 \times I_{k-2}) / \Gamma,$$

where \mathcal{R}_{k-2} a complete set of representatives of the orbits of I_{k-2}

- For $Q\in \Gamma R$, let $\gamma_Q\in \Gamma$ be an operation for which $\gamma_Q R=Q$

Symmetry reduction

Lemma (L-Machado-Oliveira-Vallentin 2018) If I_{k-2}/Γ is finite, then we have the homeomorphism

$$\prod_{R \in \mathcal{R}_{k-2}} V^2 / \operatorname{Stab}_{\Gamma}(R) \simeq (V^2 \times I_{k-2}) / \Gamma,$$

where \mathcal{R}_{k-2} a complete set of representatives of the orbits of I_{k-2}

- For $Q \in \Gamma R$, let $\gamma_Q \in \Gamma$ be an operation for which $\gamma_Q R = Q$ Corollary

If I_{k-2}/Γ is finite, then we have the isomorphism

$$\Psi \colon \bigoplus_{R \in \mathcal{R}_{k-2}} \mathcal{C}(V^2)^{\operatorname{Stab}_{\Gamma}(R)} \to \mathcal{C}(V^2 \times I_{k-2})^{\Gamma}$$

given by $\Psi(K)(x,y,Q) = K_{\gamma_Q^{-1}Q}(\gamma_Q^{-1}x,\gamma_Q^{-1}y)$

Stabilizer invariant kernels

- Let $R \in \mathcal{R}_{k-2}$ with $k \leq n$; assume vectors in R independent

Stabilizer invariant kernels

- Let $R \in \mathcal{R}_{k-2}$ with $k \leq n$; assume vectors in R independent
- Let A_R be an $n \times m$ matrix with the vectors of R as columns

Stabilizer invariant kernels

- Let $R \in \mathcal{R}_{k-2}$ with $k \leq n$; assume vectors in R independent
- Let A_R be an n imes m matrix with the vectors of R as columns
- Let $L_{A_R} = L^{-1}A_R^{\mathsf{T}}$, where L is a matrix such that LL^{T} is the Cholesky factorization of $A_R^{\mathsf{T}}A_R$
Stabilizer invariant kernels

- Let $R \in \mathcal{R}_{k-2}$ with $k \leq n$; assume vectors in R independent
- Let A_R be an n imes m matrix with the vectors of R as columns
- Let $L_{A_R} = L^{-1}A_R^{\mathsf{T}}$, where L is a matrix such that LL^{T} is the Cholesky factorization of $A_R^{\mathsf{T}}A_R$

Theorem (Musin 2014 / Nonorthogonal extension LMOV 2018) *Every*

$$K \in \mathcal{C}(S^{n-1} \times S^{n-1})^{\operatorname{Stab}_{O(n)}(\operatorname{span}(R))}_{\succeq 0}$$

can be approximated uniformly by kernels of the form

$$K(x,y) = \sum_{l=0}^{d} \operatorname{trace}(F_l Y_l^{n,m}(x \cdot y, L_{A_R}x, L_{A_R}y)),$$

where the matrices F_l are positive semidefinite

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite
- If Γ acts transitively on V, then I_{k-2}/Γ is finite for k=2,3

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite
- If Γ acts transitively on V, then I_{k-2}/Γ is finite for k=2,3
- Explains why the Delsarte and Bachoc-Vallentin bounds can be computed for spherical codes, and why it's not clear how to compute 4-point bounds for spherical codes via this approach

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite
- If Γ acts transitively on V, then I_{k-2}/Γ is finite for k=2,3
- Explains why the Delsarte and Bachoc-Vallentin bounds can be computed for spherical codes, and why it's not clear how to compute 4-point bounds for spherical codes via this approach
- For finite spherical distance graphs we do not need SOS techniques

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite
- If Γ acts transitively on V, then I_{k-2}/Γ is finite for k=2,3
- Explains why the Delsarte and Bachoc-Vallentin bounds can be computed for spherical codes, and why it's not clear how to compute 4-point bounds for spherical codes via this approach
- For finite spherical distance graphs we do not need SOS techniques
- Implementation of $\Delta_k(G)^*$ for finite spherical distance graphs for general k

- We can write $\Delta_k(G)^*$ as an SDP when I_{k-2}/Γ is finite
- If Γ acts transitively on V, then I_{k-2}/Γ is finite for k=2,3
- Explains why the Delsarte and Bachoc-Vallentin bounds can be computed for spherical codes, and why it's not clear how to compute 4-point bounds for spherical codes via this approach
- For finite spherical distance graphs we do not need SOS techniques
- Implementation of $\Delta_k(G)^*$ for finite spherical distance graphs for general k
- Currently computations for k = 4, 5









Definition (L-Vallentin 2015): $las_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\geq 0}, \\ A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\}$

Definition (L-Vallentin 2015):

$$\begin{aligned} & \log_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\geq 0}, \\ & A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \\ & A_t \colon \mathcal{C}(I_t \times I_t) \to \mathcal{C}(I_{2t}), A_t K(S) = \sum_{J, J' \in I_t \colon J \cup J' = S} K(J, J') \end{aligned}$$

Definition (L-Vallentin 2015):

$$\begin{aligned} & \log_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ & A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \\ & A_t \colon \mathcal{C}(I_t \times I_t) \to \mathcal{C}(I_{2t}), A_t K(S) = \sum_{J,J' \in I_t \colon J \cup J' = S} K(J, J') \end{aligned}$$

- $\alpha(G) \leq \operatorname{las}_t(G)^*$ for all compact topological packing graphs G

Definition (L-Vallentin 2015):

$$\begin{aligned} & \log_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ & A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \\ & A_t \colon \mathcal{C}(I_t \times I_t) \to \mathcal{C}(I_{2t}), A_t K(S) = \sum_{J,J' \in I_t \colon J \cup J' = S} K(J, J') \end{aligned}$$

- $\alpha(G) \leq \operatorname{las}_t(G)^*$ for all compact topological packing graphs G- $\operatorname{las}_t(G)^*$ is a 2t-point bound

Definition (L-Vallentin 2015):

$$las_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\}$$

$$A_t \colon \mathcal{C}(I_t \times I_t) \to \mathcal{C}(I_{2t}), A_t K(S) = \sum_{J,J' \in I_t : J \cup J' = S} K(J,J')$$

- $\alpha(G) \leq \operatorname{las}_t(G)^*$ for all compact topological packing graphs G
- $\operatorname{las}_t(G)^*$ is a 2t-point bound

Theorem

Convergence: $las_{\alpha(G)}(G)^* = \alpha(G)$

Definition (L-Vallentin 2015):

$$las_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\}$$

$$A_t \colon \mathcal{C}(I_t \times I_t) \to \mathcal{C}(I_{2t}), A_t K(S) = \sum_{J,J' \in I_t : J \cup J' = S} K(J,J')$$

- $\alpha(G) \leq \operatorname{las}_t(G)^*$ for all compact topological packing graphs G
- $\operatorname{las}_t(G)^*$ is a 2t-point bound

Theorem

Convergence: $las_{\alpha(G)}(G)^* = \alpha(G)$ (The proof uses the primal)

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

The following optimization problem gives a lower bound on the ground state energy of N particles in V with pair potential f:

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, \ K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound
- E_2^* conjectured to be universally sharp for N=5 on S^2

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound
- E_2^* conjectured to be universally sharp for N=5 on S^2
- Computational approach: Harmonic Analysis/SOS/SDP

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \leq f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound
- E_2^* conjectured to be universally sharp for N=5 on S^2
- Computational approach: Harmonic Analysis/SOS/SDP
- Numerically verified with high precision SDP solver for, e.g., the Riesz s-potentials with $s=1,\ldots,7$

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, \ K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound
- E_2^* conjectured to be universally sharp for ${\cal N}=5$ on S^2
- Computational approach: Harmonic Analysis/SOS/SDP
- Numerically verified with high precision SDP solver for, e.g., the Riesz s-potentials with $s=1,\ldots,7$
- N = 5 particularly interesting because of the phase transition

$$E_t^* = \sup\left\{\sum_{i=0}^{2t} \binom{N}{i} a_i : a \in \mathbb{R}^{\{0,\dots,2t\}}, K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ a_i + A_t K(S) \le f(S) \\ \text{for } S \in I_{=i} \text{ and } i = 0,\dots,2t\right\}$$

- Finite convergence: E_N^\ast is equal to the ground state energy
- E_1^* is essentially the Yudin bound
- E_2^* conjectured to be universally sharp for ${\cal N}=5$ on S^2
- Computational approach: Harmonic Analysis/SOS/SDP
- Numerically verified with high precision SDP solver for, e.g., the Riesz s-potentials with $s=1,\ldots,7$
- N = 5 particularly interesting because of the phase transition
- See Schwartz' talk on Friday for his approach that solves this problem for all *s* in an interval containing the phase transition

$$\begin{aligned} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{aligned}$$

$$\begin{split} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{split}$$

- May assume K is O(n)-invariant

$$\begin{aligned} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{aligned}$$

- May assume K is O(n)-invariant
- Again only finitely many linear constraints (one for each orbit)

$$\begin{aligned} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{aligned}$$

- May assume K is O(n)-invariant
- Again only finitely many linear constraints (one for each orbit)
- Need to describe the cone $\mathcal{C}(I_t \times I_t)_{\succ 0}^{O(n)}$

$$\begin{aligned} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{aligned}$$

- May assume K is O(n)-invariant
- Again only finitely many linear constraints (one for each orbit)
- Need to describe the cone $\mathcal{C}(I_t \times I_t)_{\succeq 0}^{O(n)}$
- Fourier inversion: $K(J,J') = \sum_{\pi} \operatorname{trace}(F_{\pi}Z_{\pi}(J,J'))$

$$\begin{aligned} \operatorname{las}_t(G)^* &= \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) &\leq -1_{I_{=1}}(S) \text{ for } S \in I'_{2t} \right\} \end{aligned}$$

- May assume K is O(n)-invariant
- Again only finitely many linear constraints (one for each orbit)
- Need to describe the cone $\mathcal{C}(I_t \times I_t)^{O(n)}_{\succeq 0}$
- Fourier inversion: $K(J,J') = \sum_{\pi} \operatorname{trace}(F_{\pi}Z_{\pi}(J,J'))$
- Need to compute the zonal matrices $Z_{\pi}(J,J')$

- Decompose into O(n)-irreducibles: $C(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$

- Decompose into O(n)-irreducibles: $C(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$
- Compatible orthonormal bases: $H_{\pi,i} = \operatorname{span}\{e_{\pi,i,1}, \dots, e_{\pi,i,d_{\pi}}\}$

- Decompose into O(n)-irreducibles: $C(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$
- Compatible orthonormal bases: $H_{\pi,i} = \operatorname{span}\{e_{\pi,i,1}, \dots, e_{\pi,i,d_{\pi}}\}$
- Addition formula:

$$Z_{\pi}(J,J')_{i,i'} = \sum_{j} e_{\pi,i,j}(J) \overline{e_{\pi,i,j}(J')}.$$

- Decompose into O(n)-irreducibles: $C(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$
- Compatible orthonormal bases: $H_{\pi,i} = \operatorname{span}\{e_{\pi,i,1}, \dots, e_{\pi,i,d_{\pi}}\}$
- Addition formula:

$$Z_{\pi}(J,J')_{i,i'} = \sum_{j} e_{\pi,i,j}(J)\overline{e_{\pi,i,j}(J')}.$$

- Can automate this using integration over compact groups

- Decompose into O(n)-irreducibles: $C(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$
- Compatible orthonormal bases: $H_{\pi,i} = \operatorname{span}\{e_{\pi,i,1}, \dots, e_{\pi,i,d_{\pi}}\}$
- Addition formula:

$$Z_{\pi}(J,J')_{i,i'} = \sum_{j} e_{\pi,i,j}(J)\overline{e_{\pi,i,j}(J')}.$$

- Can automate this using integration over compact groups
- Slow for large n
Approach via the addition formula

- Decompose into O(n)-irreducibles: $\mathcal{C}(I_t) = \bigoplus_{\pi} \bigoplus_{i=1}^{m_{\pi}} H_{\pi,i}$
- Compatible orthonormal bases: $H_{\pi,i} = \operatorname{span}\{e_{\pi,i,1}, \dots, e_{\pi,i,d_{\pi}}\}$
- Addition formula:

$$Z_{\pi}(J,J')_{i,i'} = \sum_{j} e_{\pi,i,j}(J)\overline{e_{\pi,i,j}(J')}.$$

- Can automate this using integration over compact groups
- Slow for large n
- This is like generating all spherical harmonics if you only need the Jacobi polynomials

- Let $\operatorname{Hom}_{O(n)}(I_t, H_{\pi})$ be the space of continuous O(n)-equivariant maps $I_t \to H_{\pi}$

- Let $\operatorname{Hom}_{O(n)}(I_t, H_\pi)$ be the space of continuous O(n)-equivariant maps $I_t \to H_\pi$
- Let $\{\varphi_i^\pi\}$ be a basis of this space

- Let ${\rm Hom}_{O(n)}(I_t,H_\pi)$ be the space of continuous $O(n)\text{-equivariant maps }I_t\to H_\pi$
- Let $\{ \varphi_i^\pi \}$ be a basis of this space
- Then, $Z_{\pi}(J,J')_{i,i'}=\left\langle \varphi_{i}^{\pi}(J),\varphi_{i'}^{\pi}(J')
 ight
 angle$

- Let ${\rm Hom}_{O(n)}(I_t,H_\pi)$ be the space of continuous $O(n)\text{-equivariant maps }I_t\to H_\pi$
- Let $\{ \varphi_i^\pi \}$ be a basis of this space
- Then, $Z_{\pi}(J,J')_{i,i'} = \left< \varphi_i^{\pi}(J), \varphi_{i'}^{\pi}(J') \right>$
- We have

$$\operatorname{Hom}_{O(n)}(I_t, H_{\pi}) \simeq \bigoplus_{R \in \mathcal{R}_t} H_{\pi}^{\operatorname{Stab}_{O(n)}(R)}$$

where \mathcal{R}_t is a complete set of representatives of the orbits

- Let ${\rm Hom}_{O(n)}(I_t,H_\pi)$ be the space of continuous $O(n)\text{-equivariant maps }I_t\to H_\pi$
- Let $\{ \varphi_i^\pi \}$ be a basis of this space
- Then, $Z_{\pi}(J,J')_{i,i'} = \left< \varphi_i^{\pi}(J), \varphi_{i'}^{\pi}(J') \right>$
- We have

$$\operatorname{Hom}_{O(n)}(I_t, H_{\pi}) \simeq \bigoplus_{R \in \mathcal{R}_t} H_{\pi}^{\operatorname{Stab}_{O(n)}(R)}$$

where \mathcal{R}_t is a complete set of representatives of the orbits

- Find the right representations H_{π} of O(n)

- Let ${\rm Hom}_{O(n)}(I_t,H_\pi)$ be the space of continuous O(n)-equivariant maps $I_t\to H_\pi$
- Let $\{ \varphi_i^\pi \}$ be a basis of this space
- Then, $Z_{\pi}(J,J')_{i,i'} = \left< \varphi_i^{\pi}(J), \varphi_{i'}^{\pi}(J') \right>$
- We have

$$\operatorname{Hom}_{O(n)}(I_t, H_{\pi}) \simeq \bigoplus_{R \in \mathcal{R}_t} H_{\pi}^{\operatorname{Stab}_{O(n)}(R)}$$

where \mathcal{R}_t is a complete set of representatives of the orbits

- Find the right representations H_{π} of O(n)
- We are essentially interested in

$$H^{SO(n-i)}_{\pi}$$
 for $i=0,\ldots,t$

where π is a representation of SO(n)

- By Frobenius reciprocity we have

$$\dim(H_{\pi}^{SO(n-t)}) = \operatorname{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$$

- By Frobenius reciprocity we have

$$\dim(H_{\pi}^{SO(n-t)}) = \mathrm{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$$

- SO(n)/SO(n-t) is a Stiefel manifold

- By Frobenius reciprocity we have

 $\dim(H_{\pi}^{SO(n-t)}) = \operatorname{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$

- SO(n)/SO(n-t) is a Stiefel manifold
- Using the branching rules of the special orthogonal groups we see that for 2t < n we can index the representations π with $m_{\pi} \neq 0$ by nonincreasing vectors $\lambda \in \mathbb{N}_0^t$

- By Frobenius reciprocity we have

 $\dim(H_{\pi}^{SO(n-t)}) = \operatorname{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$

- SO(n)/SO(n-t) is a Stiefel manifold
- Using the branching rules of the special orthogonal groups we see that for 2t < n we can index the representations π with $m_{\pi} \neq 0$ by nonincreasing vectors $\lambda \in \mathbb{N}_0^t$
- The polynomial representations ρ of $\mathrm{GL}(t)$ can also be indexed by such vectors!

- By Frobenius reciprocity we have

 $\dim(H_{\pi}^{SO(n-t)}) = \operatorname{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$

- SO(n)/SO(n-t) is a Stiefel manifold
- Using the branching rules of the special orthogonal groups we see that for 2t < n we can index the representations π with $m_{\pi} \neq 0$ by nonincreasing vectors $\lambda \in \mathbb{N}_0^t$
- The polynomial representations ρ of $\mathrm{GL}(t)$ can also be indexed by such vectors!
- [Gelbart 1974] showed $m_{\pi_{\lambda}} = \dim(\rho_{\lambda})$

- By Frobenius reciprocity we have

 $\dim(H_{\pi}^{SO(n-t)}) = \operatorname{mult}(H_{\pi}, L^{2}(SO(n)/SO(n-t))) =: m_{\pi}$

- SO(n)/SO(n-t) is a Stiefel manifold
- Using the branching rules of the special orthogonal groups we see that for 2t < n we can index the representations π with $m_{\pi} \neq 0$ by nonincreasing vectors $\lambda \in \mathbb{N}_0^t$
- The polynomial representations ρ of $\mathrm{GL}(t)$ can also be indexed by such vectors!
- [Gelbart 1974] showed $m_{\pi_{\lambda}} = \dim(\rho_{\lambda})$

"seems to be an act of providence"

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in $H_{\rho_{\lambda}}$ to a function $O(n) \to H_{\rho_{\lambda}}$

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in $H_{\rho_{\lambda}}$ to a function $O(n) \rightarrow H_{\rho_{\lambda}}$
- Construct $H_{\rho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0\leq i< t$

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0\leq i< t$
- Combining this gives

$$Z_{\pi}(J,J')_{i,i'} = \int_{O(n)} \int_{U(t)} p_{\pi,i,i',J,J'}(\gamma,\xi) \, d\xi \, d\gamma,$$

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0\leq i< t$
- Combining this gives

$$Z_{\pi}(J,J')_{i,i'} = \int_{O(n)} \int_{U(t)} p_{\pi,i,i',J,J'}(\gamma,\xi) \, d\xi \, d\gamma,$$

where $p_{\pi,i,i',J,J'}$ is some explicitly computable polynomial - Outer integral is difficult in general since n is large

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0 \leq i < t$
- Combining this gives

$$Z_{\pi}(J,J')_{i,i'} = \int_{O(n)} \int_{U(t)} p_{\pi,i,i',J,J'}(\gamma,\xi) \, d\xi \, d\gamma,$$

- Outer integral is difficult in general since \boldsymbol{n} is large
- Z_{π} is O(n-t)-invariant, so we only need to evaluate Z_{π} at sets J, J' for which $p_{\pi,i,i',J,J'}$ depends on very few entries of γ

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0 \leq i < t$
- Combining this gives

$$Z_{\pi}(J,J')_{i,i'} = \int_{O(n)} \int_{U(t)} p_{\pi,i,i',J,J'}(\gamma,\xi) \, d\xi \, d\gamma,$$

- Outer integral is difficult in general since \boldsymbol{n} is large
- Z_{π} is O(n-t)-invariant, so we only need to evaluate Z_{π} at sets J,J' for which $p_{\pi,i,i',J,J'}$ depends on very few entries of γ
- [Gorin-Lopez 2008] give formula to compute the integral of a monomial over O(n) where the complexity depends only on the entries and degrees of the integrand (not on n)

- [Gross-Kunze 1977] give two isomorphisms $H_{\rho_\lambda} \to H^{SO(n-t)}_{\pi_\lambda}$
- The first maps a vector in H_{ρ_λ} to a function $O(n) \to H_{\rho_\lambda}$
- Construct $H_{
 ho_{\lambda}}$ as polynomials $\operatorname{GL}(t) \to \mathbb{C}$
- By choosing subspaces of H_{ρ_λ} we can also describe $H^{SO(n-i)}_{\pi_\lambda}$ for $0 \leq i < t$
- Combining this gives

$$Z_{\pi}(J,J')_{i,i'} = \int_{O(n)} \int_{U(t)} p_{\pi,i,i',J,J'}(\gamma,\xi) \, d\xi \, d\gamma,$$

- Outer integral is difficult in general since \boldsymbol{n} is large
- Z_{π} is O(n-t)-invariant, so we only need to evaluate Z_{π} at sets J,J' for which $p_{\pi,i,i',J,J'}$ depends on very few entries of γ
- [Gorin-Lopez 2008] give formula to compute the integral of a monomial over O(n) where the complexity depends only on the entries and degrees of the integrand (not on n)
- The implementation is work in progress

Thank you!