Semidefinite programming hierarchies for packing and energy minimization (3/4)

David de Laat (TU Delft)

Summer School on Optimization, Interpolation and Modular Forms,
August 24–28, 2020, EPFL

Topics for the four talks

1. Sums-of-squares hierarchies for polynomial optimization
2. Moment hierarchies for polynomial optimization
3. **Packing problems**
4. Energy minimization problems

Spherical code problem as graph problem

Spherical code problem: Given a dimension n and angle θ, what is the largest set $C \subseteq S^{n-1}$ with $x \cdot y \leq \cos\theta$ for all distinct $x, y \in C$

Spherical code problem as graph problem

Spherical code problem: Given a dimension n and angle θ, what is the largest set $C \subseteq S^{n-1}$ with $x \cdot y \leq \cos\theta$ for all distinct $x, y \in C$

This is an independent set problem in the graph with vertex set S^{n-1}, where two distinct vertices $x, y \in S^{n-1}$ are adjacent if $x \cdot y > \cos\theta$

Topological packing graphs

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

Topological packing graphs

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

- A clique in a graph is a subset of the vertex set where any two distinct vertices are adjacent.

Topological packing graphs

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

- A clique in a graph is a subset of the vertex set where any two distinct vertices are adjacent.
- It suffices to verify the condition for cliques of size one and two. But if we require this for all cliques (which is equivalent to requiring this for all maximal cliques), then the definition does really change.

Topological packing graphs

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

- A clique in a graph is a subset of the vertex set where any two distinct vertices are adjacent.
- It suffices to verify the condition for cliques of size one and two. But if we require this for all cliques (which is equivalent to requiring this for all maximal cliques), then the definition does really change.
- A compact topological packing graph has finite independence number.

Topological packing graphs

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

- A clique in a graph is a subset of the vertex set where any two distinct vertices are adjacent.
- It suffices to verify the condition for cliques of size one and two. But if we require this for all cliques (which is equivalent to requiring this for all maximal cliques), then the definition does really change.
- A compact topological packing graph has finite independence number.
- Why not a metric space? We do not always have a natural metric, for instance when we pack different objects (e.g., binary spherical cap packings)

Independent sets in compact topological packing graphs

Let I_t be the set of independent sets of cardinality at most t

Independent sets in compact topological packing graphs

Let I_t be the set of independent sets of cardinality at most t

$I_t \setminus \{\emptyset\}$ gets a topology by using the product topology on V^t and then the quotient topology from

$$q \colon V^t \to I_t \setminus \{\emptyset\}, (x_1, \ldots, x_t) \mapsto \{x_1, \ldots, x_t\}$$

Independent sets in compact topological packing graphs

Let I_t be the set of independent sets of cardinality at most t

$I_t \setminus \{\emptyset\}$ gets a topology by using the product topology on V^t and then the quotient topology from

$$q \colon V^t \to I_t \setminus \{\emptyset\}, (x_1, \ldots, x_t) \mapsto \{x_1, \ldots, x_t\}$$

To get I_t we add the isolated point $\emptyset$

Independent sets in compact topological packing graphs

Let I_t be the set of independent sets of cardinality at most t

$I_t \setminus \{\emptyset\}$ gets a topology by using the product topology on V^t and then the quotient topology from

$$q\colon V^t \to I_t \setminus \{\emptyset\}, (x_1, \ldots, x_t) \mapsto \{x_1, \ldots, x_t\}$$

To get I_t we add the isolated point $\emptyset$

If V has a metric, then I_t has the Hausdorff distance as metric

Independent sets in compact topological packing graphs

Let I_t be the set of independent sets of cardinality at most t

$I_t \setminus \{\emptyset\}$ gets a topology by using the product topology on V^t and then the quotient topology from

$$q\colon V^t \to I_t \setminus \{\emptyset\}, (x_1, \ldots, x_t) \mapsto \{x_1, \ldots, x_t\}$$

To get I_t we add the isolated point $\emptyset$

If V has a metric, then I_t has the Hausdorff distance as metric

For a compact topological packing graph, the set I_t is compact, and the sets $I_t \setminus I_{t-1}$ are both open and closed

Moment hierarchy for finite graphs

Moment hierarchy for the independent set problem in a finite graph:

$$P_t = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\, M_t^1(y) \succeq 0,\, y_S = 0 \text{ for } S \text{ dependent} \Big\}$$

Here we optimize over vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$.

Moment hierarchy for finite graphs

Moment hierarchy for the independent set problem in a finite graph:

$$P_t = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\ M_t^1(y) \succeq 0,\ y_S = 0 \text{ for } S \text{ dependent} \Big\}$$

Here we optimize over vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$.

This gives upper bounds: For S an independent set, the vector y given by

$$y_R = \begin{cases} 1 & \text{if } R \subseteq S, \\ 0 & \text{otherwise} \end{cases}$$

for $|R| \leq 2t$ is feasible

Moment hierarchy for finite graphs

Moment hierarchy for the independent set problem in a finite graph:

$$P_t = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\, M_t^1(y) \succeq 0,\, y_S = 0 \text{ for } S \text{ dependent} \Big\}$$

Here we optimize over vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$.

This gives upper bounds: For S an independent set, the vector y given by

$$y_R = \begin{cases} 1 & \text{if } R \subseteq S, \\ 0 & \text{otherwise} \end{cases}$$

for $|R| \leq 2t$ is feasible

$$\sum_{J,J'} c_J c_{J'} M_t^1(y)_{J,J'} = \sum_{J,J'} c_J c_{J'} y_{J \cup J'} = \left(\sum_{J \subseteq S} c_J \right)^2 \geq 0.$$

Moment hierarchy for finite graphs

Moment hierarchy for the independent set problem in a finite graph:

$$P_t = \sup\left\{ \sum_{i=1}^n y_{\{i\}} : y_\emptyset = 1,\, M_t^1(y) \succeq 0,\, y_S = 0 \text{ for } S \text{ dependent}\right\}$$

Here we optimize over vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$.

This gives upper bounds: For S an independent set, the vector y given by

$$y_R = \begin{cases} 1 & \text{if } R \subseteq S, \\ 0 & \text{otherwise} \end{cases}$$

for $|R| \leq 2t$ is feasible

$$\sum_{J,J'} c_J c_{J'} M_t^1(y)_{J,J'} = \sum_{J,J'} c_J c_{J'} y_{J \cup J'} = \left(\sum_{J \subseteq S} c_J\right)^2 \geq 0.$$

This also shows we can add the constraint that y is entrywise nonnegative

Convergence in $\alpha(G)$ steps

Proposition (Lindström and Wilf) The cone of positive semidefinite moment matrices is

$$\text{cone}\{\chi_S(\chi_S)^{\mathsf{T}} : S \subseteq \{1, \ldots, n\}\}$$

Convergence in $\alpha(G)$ steps

Proposition (Lindström and Wilf) The cone of positive semidefinite moment matrices is

$$\text{cone}\{\chi_S(\chi_S)^{\mathsf{T}} : S \subseteq \{1,\ldots,n\}\}$$

Here moment matrices are matrices of the form $M_t^1(y)$ for y a vector indexed by all subsets of $\{1,\ldots,n\}$.

Convergence in $\alpha(G)$ steps

Proposition (Lindström and Wilf) The cone of positive semidefinite moment matrices is

$$\text{cone}\{\chi_S(\chi_S)^{\mathsf{T}} : S \subseteq \{1, \ldots, n\}\}$$

Here moment matrices are matrices of the form $M_t^1(y)$ for y a vector indexed by all subsets of $\{1, \ldots, n\}$.

Laurent uses this to give a direct proof for convergence of the moment hierarchy for $0/1$ polynomial optimization problems in at most n steps.

Convergence in $\alpha(G)$ steps

Proposition (Lindström and Wilf) The cone of positive semidefinite moment matrices is

$$\mathrm{cone}\{\chi_S(\chi_S)^{\mathsf{T}} : S \subseteq \{1, \ldots, n\}\}$$

Here moment matrices are matrices of the form $M_t^1(y)$ for y a vector indexed by all subsets of $\{1, \ldots, n\}$.

Laurent uses this to give a direct proof for convergence of the moment hierarchy for $0/1$ polynomial optimization problems in at most n steps.

The moment hierarchy for the independent set problem does not change anymore for $t \geq \alpha(G)$, so we get convergence in $\alpha(G)$ steps

Convergence in $\alpha(G)$ steps

Proposition (Lindström and Wilf) The cone of positive semidefinite moment matrices is

$$\text{cone}\{\chi_S(\chi_S)^{\mathsf{T}} : S \subseteq \{1, \ldots, n\}\}$$

Here moment matrices are matrices of the form $M_t^1(y)$ for y a vector indexed by all subsets of $\{1, \ldots, n\}$.

Laurent uses this to give a direct proof for convergence of the moment hierarchy for $0/1$ polynomial optimization problems in at most n steps.

The moment hierarchy for the independent set problem does not change anymore for $t \geq \alpha(G)$, so we get convergence in $\alpha(G)$ steps

Exercise 7 Use the result by Lindström and Wilf to give a direct proof for the convergence of the moment hierachy for the independent set problem.

Extension to infinite graphs

$$P'_t = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\ M_t^1(y) \succeq 0,\ y_S = 0 \text{ for } S \text{ dependent},\ y \geq 0 \Big\}$$

For finite graphs we optimize over entrywise nonnegative vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$ with $y_S = 0$ for S dependent

Extension to infinite graphs

$$P_t' = \sup\left\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\ M_t^1(y) \succeq 0,\ y_S = 0 \text{ for } S \text{ dependent},\ y \geq 0 \right\}$$

For finite graphs we optimize over entrywise nonnegative vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$ with $y_S = 0$ for S dependent

For infinite graphs we will optimize over positive measures λ on I_{2t}

Extension to infinite graphs

$$P_t' = \sup \left\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\, M_t^1(y) \succeq 0,\, y_S = 0 \text{ for } S \text{ dependent},\, y \geq 0 \right\}$$

For finite graphs we optimize over entrywise nonnegative vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$ with $y_S = 0$ for S dependent

For infinite graphs we will optimize over positive measures λ on I_{2t}

The normalization condition becomes $\lambda(\{\emptyset\}) = 1$

Extension to infinite graphs

$$P_t' = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\, M_t^1(y) \succeq 0,\, y_S = 0 \text{ for } S \text{ dependent},\, y \geq 0 \Big\}$$

For finite graphs we optimize over entrywise nonnegative vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$ with $y_S = 0$ for S dependent

For infinite graphs we will optimize over positive measures λ on I_{2t}

The normalization condition becomes $\lambda(\{\emptyset\}) = 1$

The objective becomes $\lambda(I_1 \setminus \{\emptyset\})$

Extension to infinite graphs

$$P_t' = \sup \Big\{ \sum_{i=1}^{n} y_{\{i\}} : y_\emptyset = 1,\ M_t^1(y) \succeq 0,\ y_S = 0 \text{ for } S \text{ dependent},\ y \geq 0 \Big\}$$

For finite graphs we optimize over entrywise nonnegative vectors y indexed by subsets of $\{1, \ldots, n\}$ of cardinality at most $2t$ with $y_S = 0$ for S dependent

For infinite graphs we will optimize over positive measures λ on I_{2t}

The normalization condition becomes $\lambda(\{\emptyset\}) = 1$

The objective becomes $\lambda(I_1 \setminus \{\emptyset\})$

What about positive semidefiniteness of the moment matrix?

Positive semidefinite moment matrices

$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle M_t^1(y), X \rangle \geq 0$ for all $X \succeq 0$

Positive semidefinite moment matrices

$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle M_t^1(y), X \rangle \geq 0$ for all $X \succeq 0$

With A_t the adjoint of M_t^1 we have:
$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle y, A_t X \rangle \geq 0$ for all $X \succeq 0$

Positive semidefinite moment matrices

$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle M_t^1(y), X\rangle \geq 0$ for all $X \succeq 0$

With A_t the adjoint of M_t^1 we have:
$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle y, A_t X\rangle \geq 0$ for all $X \succeq 0$

For infinite graphs we have

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

Positive semidefinite moment matrices

$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle M_t^1(y), X\rangle \geq 0$ for all $X \succeq 0$

With A_t the adjoint of M_t^1 we have:
$M_t^1(y) \succeq 0 \quad \Leftrightarrow \quad \langle y, A_t X\rangle \geq 0$ for all $X \succeq 0$

For infinite graphs we have

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

The constraint $M_t^1(y) \succeq 0$ becomes

$$\lambda(A_t K) \geq 0 \quad \text{for all positive definite kernels} \quad K \in \mathcal{C}(I_t \times I_t)$$

A moment hierarchy for infinite graphs

Definition (L-Vallentin 2015)

$$\sup\Big\{\lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\ \lambda(\{\emptyset\}) = 1,$$
$$\lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t)\Big\}$$

A moment hierarchy for infinite graphs

Definition (L-Vallentin 2015)

$$\sup\Big\{\lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\ \lambda(\{\emptyset\}) = 1,$$
$$\lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t)\Big\}$$

For each t we get an upper bound on the independence number: If S is an independent set, then $\lambda = \chi_S := \sum_{R \subseteq S} \delta_R$ is feasible

A moment hierarchy for infinite graphs

Definition (L-Vallentin 2015)

$$\sup \Big\{ \lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\ \lambda(\{\emptyset\}) = 1,$$
$$\lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t) \Big\}$$

For each t we get an upper bound on the independence number: If S is an independent set, then $\lambda = \chi_S := \sum_{R \subseteq S} \delta_R$ is feasible

This generalizes the Lasserre moment hierarchy for the independent set problem; now we need to generalize Laurent's convergence proof

Möbius inversion

Lemma For each signed measure λ on I_{2t} there exists a unique signed measure σ on I_{2t} such that $\lambda = \int \chi_S \, d\sigma(S)$. If λ is supported on I_t and satisfies $\lambda(A_t K) \geq 0$ for all positive definite kernels $K \in \mathcal{C}(I_t \times I_t)$, then σ is a positive measure supported on I_t.

Möbius inversion

Lemma For each signed measure λ on I_{2t} there exists a unique signed measure σ on I_{2t} such that $\lambda = \int \chi_S \, d\sigma(S)$. If λ is supported on I_t and satisfies $\lambda(A_t K) \geq 0$ for all positive definite kernels $K \in \mathcal{C}(I_t \times I_t)$, then σ is a positive measure supported on I_t.

$$\sup \Big\{ \lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\ \lambda(\{\emptyset\}) = 1, \\ \lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t) \Big\}$$

Möbius inversion

Lemma For each signed measure λ on I_{2t} there exists a unique signed measure σ on I_{2t} such that $\lambda = \int \chi_S \, d\sigma(S)$. If λ is supported on I_t and satisfies $\lambda(A_t K) \geq 0$ for all positive definite kernels $K \in \mathcal{C}(I_t \times I_t)$, then σ is a positive measure supported on I_t.

$$\sup \big\{ \lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\ \lambda(\{\emptyset\}) = 1,$$
$$\lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t) \big\}$$

If t equals the independence number $\alpha(G)$ of the graph, then $I_t = I_{2t}$, so we can apply the above lemma to a feasible solution λ.

Möbius inversion

Lemma For each signed measure λ on I_{2t} there exists a unique signed measure σ on I_{2t} such that $\lambda = \int \chi_S \, d\sigma(S)$. If λ is supported on I_t and satisfies $\lambda(A_t K) \geq 0$ for all positive definite kernels $K \in \mathcal{C}(I_t \times I_t)$, then σ is a positive measure supported on I_t.

$$\sup \big\{ \lambda(I_1 \setminus \{\emptyset\}) : \lambda \text{ a positive measure on } I_{2t},\, \lambda(\{\emptyset\}) = 1, \\ \lambda(A_t K) \geq 0 \text{ for all positive definite kernels } K \in \mathcal{C}(I_t \times I_t) \big\}$$

If t equals the independence number $\alpha(G)$ of the graph, then $I_t = I_{2t}$, so we can apply the above lemma to a feasible solution λ.

Using the normalization condition the optimization problem reduces to

$$\sup \Big\{ \int \chi_S(I_1 \setminus \{\emptyset\}) \, d\sigma(S) : \sigma \in \mathcal{P}(I_{\alpha(G)}) \Big\}$$

which is equal to $\alpha(G)$

The dual hierarchy

Conic duality shows the dual hierarchy is given by

$$\inf \Big\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t) \text{ positive definite}, \\ A_t K(S) \leq -1 \text{ for } S \in I_1 \setminus \{\emptyset\}, \\ A_t K(S) \leq 0 \text{ for } S \in I_{2t} \setminus I_1 \Big\}$$

The dual hierarchy

Conic duality shows the dual hierarchy is given by

$$\begin{aligned}\inf \Big\{ K(\emptyset,\emptyset) : \; & K \in \mathcal{C}(I_t \times I_t) \text{ positive definite}, \\ & A_t K(S) \leq -1 \text{ for } S \in I_1 \setminus \{\emptyset\}, \\ & A_t K(S) \leq 0 \text{ for } S \in I_{2t} \setminus I_1 \Big\}\end{aligned}$$

For each t weak duality shows this gives an upper bound on the corresponding problem in the moment hierarchy, and hence an upper bound on the independence number

The dual hierarchy

Conic duality shows the dual hierarchy is given by

$$\inf \Big\{ K(\emptyset,\emptyset) : K \in \mathcal{C}(I_t \times I_t) \text{ positive definite}, \\ A_t K(S) \leq -1 \text{ for } S \in I_1 \setminus \{\emptyset\}, \\ A_t K(S) \leq 0 \text{ for } S \in I_{2t} \setminus I_1 \Big\}$$

For each t weak duality shows this gives an upper bound on the corresponding problem in the moment hierarchy, and hence an upper bound on the independence number

In fact, strong duality holds, so in principle we can solve any compact packing problem up to any precision by solving these dual problems.

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

Lovász sandwhich theorem: It upper bounds the independence number $\alpha(G)$ and lower bounds the chromatic number of the complement graph

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

Lovász sandwhich theorem: It upper bounds the independence number $\alpha(G)$ and lower bounds the chromatic number of the complement graph

It also upper bounds the Shannon capacity of a graph

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

Lovász sandwhich theorem: It upper bounds the independence number $\alpha(G)$ and lower bounds the chromatic number of the complement graph

It also upper bounds the Shannon capacity of a graph

For finite graphs it is a semidefinite program

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

Lovász sandwhich theorem: It upper bounds the independence number $\alpha(G)$ and lower bounds the chromatic number of the complement graph

It also upper bounds the Shannon capacity of a graph

For finite graphs it is a semidefinite program

For infinite graphs the theta' number it can be written as

$$\begin{aligned}\inf \Big\{ a : a \in \mathbb{R},\, F \in \mathcal{C}(V \times V) \text{ positive definite},\\ F(x,x) \leq a - 1 \text{ for } x \in V,\\ F(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.\end{aligned}$$

The Lovász theta number

The Lovász theta number is an important graph parameter in combinatorial optimization

Lovász sandwhich theorem: It upper bounds the independence number $\alpha(G)$ and lower bounds the chromatic number of the complement graph

It also upper bounds the Shannon capacity of a graph

For finite graphs it is a semidefinite program

For infinite graphs the theta' number it can be written as

$$\inf \Big\{ a : a \in \mathbb{R},\, F \in \mathcal{C}(V \times V) \text{ positive definite}, \\ F(x,x) \leq a - 1 \text{ for } x \in V, \\ F(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

Using the Schur complement it follows this is the first step of the dual hierarchy

Delsarte bound

The theta' number:

$$\inf \Big\{ a : a \in \mathbb{R},\ K \in \mathcal{C}(S^{n-1} \times S^{n-1}) \text{ positive definite}, \\ K(x,x) \le a - 1 \text{ for } x \in V, \\ K(x,y) \le -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

Delsarte bound

The theta' number:

$$\inf \Big\{ a : a \in \mathbb{R},\, K \in \mathcal{C}(S^{n-1} \times S^{n-1}) \text{ positive definite,}$$
$$K(x,x) \le a - 1 \text{ for } x \in V,$$
$$K(x,y) \le -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

As observed by Bachoc, Nebe, Oliveira, Vallentin the theta' number for the sphere reduces to the Delsarte bound

Delsarte bound

The theta' number:

$$\inf \Big\{ a : a \in \mathbb{R},\ K \in \mathcal{C}(S^{n-1} \times S^{n-1}) \text{ positive definite}, \\ K(x,x) \leq a - 1 \text{ for } x \in V, \\ K(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

As observed by Bachoc, Nebe, Oliveira, Vallentin the theta' number for the sphere reduces to the Delsarte bound

We may assume K to be $O(n)$ invariant; that is, $K(Ax, Ay) = K(x, y)$ for all $A \in O(n)$ and $x, y \in S^{n-1}$

Delsarte bound

The theta' number:

$$\inf \Big\{ a : a \in \mathbb{R},\ K \in \mathcal{C}(S^{n-1} \times S^{n-1}) \text{ positive definite}, \\ K(x,x) \leq a - 1 \text{ for } x \in V, \\ K(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

As observed by Bachoc, Nebe, Oliveira, Vallentin the theta' number for the sphere reduces to the Delsarte bound

We may assume K to be $O(n)$ invariant; that is, $K(Ax, Ay) = K(x,y)$ for all $A \in O(n)$ and $x, y \in S^{n-1}$

If (a, K) is feasible, then $(a, \bar{K})$ is also feasible, where

$$\bar{K}(x,y) = \int_{O(n)} K(Ax, Ay)\, dA$$

(integration is over the normalized Haar measure)

Delsarte bound

Schoenberg's theorem If K is an $O(n)$-invariant, positive definite kernel $K \in \mathcal{C}(S^{n-1} \times S^{n-1})$, then

$$K(x, y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y)$$

with $c_k \geq 0$, where convergence is uniform absolute. Here P_k^n is the ultraspherical polynomial of degree k in dimension n

Delsarte bound

Schoenberg's theorem If K is an $O(n)$-invariant, positive definite kernel $K \in \mathcal{C}(S^{n-1} \times S^{n-1})$, then

$$K(x, y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y)$$

with $c_k \geq 0$, where convergence is uniform absolute. Here P_k^n is the ultraspherical polynomial of degree k in dimension n

This shows theta' reduces to

$$\begin{aligned}\inf \Big\{ a : a \in \mathbb{R},\ K(x, y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y),& \\ c_0, c_1, \ldots \geq 0,& \\ K(x, x) \leq a - 1 \text{ for } x \in V,& \\ K(x, y) \leq -1 \text{ for } \{x, y\} \in I_{=2} \Big\}.&\end{aligned}$$

Delsarte bound

This shows theta' reduces to

$$\inf \Big\{ a : a \in \mathbb{R},\ K(x,y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y),$$
$$c_0, c_1, \ldots \geq 0,$$
$$K(x,x) \leq a - 1 \text{ for } x \in V,$$
$$K(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

Delsarte bound

This shows theta' reduces to

$$\inf \Big\{ a : a \in \mathbb{R},\ K(x,y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y),$$
$$c_0, c_1, \ldots \geq 0,$$
$$K(x,x) \leq a - 1 \text{ for } x \in V,$$
$$K(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

Replacing $x \cdot y$ by u gives

$$\inf \Big\{ a : a \in \mathbb{R},\ f(u) = \sum_{k=0}^{\infty} c_k P_k^n(u),$$
$$c_0, c_1, \ldots \geq 0,$$
$$f(1) \leq a - 1 \text{ for } x \in V,$$
$$f(u) \leq -1 \text{ for } u \in [\cos\theta, 1] \Big\}.$$

Delsarte bound

This shows theta' reduces to

$$\inf \Big\{ a : a \in \mathbb{R},\ K(x,y) = \sum_{k=0}^{\infty} c_k P_k^n(x \cdot y),\\ c_0, c_1, \ldots \geq 0,\\ K(x,x) \leq a - 1 \text{ for } x \in V,\\ K(x,y) \leq -1 \text{ for } \{x,y\} \in I_{=2} \Big\}.$$

Replacing $x \cdot y$ by u gives

$$\inf \Big\{ a : a \in \mathbb{R},\ f(u) = \sum_{k=0}^{\infty} c_k P_k^n(u),\\ c_0, c_1, \ldots \geq 0,\\ f(1) \leq a - 1 \text{ for } x \in V,\\ f(u) \leq -1 \text{ for } u \in [\cos\theta, 1] \Big\}.$$

By removing a from the problem we recover the Delsarte linear programming bound.