Energy minimization via conic programming hierarchies

David de Laat (TU Delft)

SIAM conference on optimization
May 20, 2014, San Diego

Energy minimization

Given

- a set V (container)
- a function $w\colon V \times V \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ (pair potential)
- an integer N (number of particles)

What is the minimal potential energy of a particle configuration?

Energy minimization

Given

- a set V (container)
- a function $w\colon V \times V \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ (pair potential)
- an integer N (number of particles)

What is the minimal potential energy of a particle configuration?

$$E = \inf_{S \in \binom{V}{N}} \sum_{\{x,y\} \in \binom{S}{2}} w(x, y)$$

Energy minimization

Given

- a set V (container)
- a function $w\colon V \times V \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ (pair potential)
- an integer N (number of particles)

What is the minimal potential energy of a particle configuration?

$$E = \inf_{S \in \binom{V}{N}} \sum_{\{x,y\} \in \binom{S}{2}} w(x,y)$$

Example

For the Thomson problem we take $V = S^2$ and $w(x,y) = \|x-y\|^{-1}$

Lower bounds

- Configurations provide upper bounds on the optimal energy E

Lower bounds

- Configurations provide upper bounds on the optimal energy E
- Usually hard to prove optimality of a configuration

Lower bounds

- Configurations provide upper bounds on the optimal energy E
- Usually hard to prove optimality of a configuration

Approach to finding lower bounds

1. Relax the problem to a conic optimization problem
2. Find good feasible solutions to the dual problem

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints
- Relaxation: instead of optimizing over N-particle subsets, optimize over functions satisfying these constraints

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints
- Relaxation: instead of optimizing over N-particle subsets, optimize over functions satisfying these constraints
- 2-point bounds using contraints from positive Γ-invariant kernels on V [Yudin 1992]

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints
- Relaxation: instead of optimizing over N-particle subsets, optimize over functions satisfying these constraints
- 2-point bounds using contraints from positive Γ-invariant kernels on V [Yudin 1992]
- Universal optimality of configurations using 2-point bounds [Cohn-Kumar 2006]

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints
- Relaxation: instead of optimizing over N-particle subsets, optimize over functions satisfying these constraints
- 2-point bounds using contraints from positive Γ-invariant kernels on V [Yudin 1992]
- Universal optimality of configurations using 2-point bounds [Cohn-Kumar 2006]
- 3-point using constraints from kernels which are invariant under the stabilizer subgroup of a point [Schrijver 2005, Bachoc-Vallentin 2009, Cohn-Woo 2012]

Related work

- The symmetry group Γ of V acts on V^k by $\gamma(x_1, \ldots, x_k) = (\gamma x_1, \ldots, \gamma x_k)$
- The k-point correlation function of a configuration $S \subseteq V$ measures the number of k-subsets of S in each orbit in V^k
- These functions satisfy certain linear/semidefinite constraints
- Relaxation: instead of optimizing over N-particle subsets, optimize over functions satisfying these constraints
- 2-point bounds using contraints from positive Γ-invariant kernels on V [Yudin 1992]
- Universal optimality of configurations using 2-point bounds [Cohn-Kumar 2006]
- 3-point using constraints from kernels which are invariant under the stabilizer subgroup of a point [Schrijver 2005, Bachoc-Vallentin 2009, Cohn-Woo 2012]
- k-point bounds using the stabilizer subgroup of $k-2$ points [Musin 2007]

This talk

- Hierarchy for energy minimization based on a generalization by [L.-Vallentin 2013] of the Lasserre hierarchy for the independent set problem to infinite graphs

This talk

- Hierarchy for energy minimization based on a generalization by [L.-Vallentin 2013] of the Lasserre hierarchy for the independent set problem to infinite graphs
- Instead of correlation functions we have "correlation measures", and instead of positive kernels invariant under a stabilizer subgroup we have positive kernels on subset spaces

This talk

- Hierarchy for energy minimization based on a generalization by [L.-Vallentin 2013] of the Lasserre hierarchy for the independent set problem to infinite graphs
- Instead of correlation functions we have "correlation measures", and instead of positive kernels invariant under a stabilizer subgroup we have positive kernels on subset spaces
- Convergent hierarchy of *finite* semidefinite programs

This talk

- Hierarchy for energy minimization based on a generalization by [L.-Vallentin 2013] of the Lasserre hierarchy for the independent set problem to infinite graphs
- Instead of correlation functions we have "correlation measures", and instead of positive kernels invariant under a stabilizer subgroup we have positive kernels on subset spaces
- Convergent hierarchy of *finite* semidefinite programs
- Application to low dimensional spaces

Setup

Restrict to particle configurations whose points are not “too close”:

Setup

Restrict to particle configurations whose points are not “too close”:

- Assume V is a compact Hausdorff space

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w \colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x,y) \to \infty$ as (x,y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x,y) > \delta$$

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x, y) > \delta$$

- Consider only *independent sets* in G of cardinality N

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x, y) > \delta$$

- Consider only *independent sets* in G of cardinality N

Subset spaces:

Setup

Restrict to particle configurations whose points are not “too close”:

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x, y) > \delta$$

- Consider only *independent sets* in G of cardinality N

Subset spaces:

- Let V_t be the set of subsets of V of cardinality at most t with topology induced by $q\colon V^t \to V_t$, $(v_1, \ldots, v_t) \mapsto \{v_1, \ldots, v_t\}$

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x, y) > \delta$$

- Consider only *independent sets* in G of cardinality N

Subset spaces:

- Let V_t be the set of subsets of V of cardinality at most t with topology induced by $q\colon V^t \to V_t$, $(v_1, \ldots, v_t) \mapsto \{v_1, \ldots, v_t\}$
- Denote by $I_t \subset V_t$ the compact subset of independent sets

Setup

Restrict to particle configurations whose points are not "too close":

- Assume V is a compact Hausdorff space
- Assume $w\colon V \times V \setminus \Delta_V \to \mathbb{R}$ is a continuous function with $w(x, y) \to \infty$ as (x, y) converges to the diagonal
- Let $\delta > E$ and define the graph $G = (V, E)$ where

$$x \sim y \text{ if } w(x, y) > \delta$$

- Consider only *independent sets* in G of cardinality N

Subset spaces:

- Let V_t be the set of subsets of V of cardinality at most t with topology induced by $q\colon V^t \to V_t$, $(v_1, \ldots, v_t) \mapsto \{v_1, \ldots, v_t\}$
- Denote by $I_t \subset V_t$ the compact subset of independent sets
- View w as an element in $\mathcal{C}(I_{2t})$

Primal hierarchy

- We define a hierarchy of conic optimization problems with optimal values $E_1, E_2, \ldots$ such that

$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

Primal hierarchy

- We define a hierarchy of conic optimization problems with optimal values $E_1, E_2, \ldots$ such that

$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- E_t is a $\min\{2t, N\}$-point bound

Primal hierarchy

- We define a hierarchy of conic optimization problems with optimal values $E_1, E_2, \ldots$ such that

$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- E_t is a $\min\{2t, N\}$-point bound
- In the t-th step: optimize over a cone $K_t(G)$ of Borel measures on $I_{\min\{2t,N\}}$

Primal hierarchy

- We define a hierarchy of conic optimization problems with optimal values $E_1, E_2, \ldots$ such that

$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- E_t is a $\min\{2t, N\}$-point bound
- In the t-th step: optimize over a cone $K_t(G)$ of Borel measures on $I_{\min\{2t,N\}}$

$$E_t = \min\Big\{\lambda(w) : \lambda \in K_t(G), \\ \lambda(I_{=i}) = \binom{N}{i} \text{ for } i = 1, \ldots, \min\{2t, N\}\Big\}$$

Primal hierarchy

- We define a hierarchy of conic optimization problems with optimal values $E_1, E_2, \ldots$ such that

$$E_1 \leq E_2 \leq \cdots \leq E_N = E$$

- E_t is a $\min\{2t, N\}$-point bound
- In the t-th step: optimize over a cone $K_t(G)$ of Borel measures on $I_{\min\{2t,N\}}$

$$E_t = \min \Big\{ \lambda(w) : \lambda \in K_t(G), \\ \lambda(I_{=i}) = \binom{N}{i} \text{ for } i = 1, \ldots, \min\{2t, N\} \Big\}$$

- If S is a N-particle configuration, then

$$\chi_S = \sum_{R \subseteq S : |R| \leq 2t} \delta_R$$

is a feasible measure (this proves $E_t \leq E$)

Cone of moment measures

- Define the operator $A_t \colon \mathcal{C}(V_t \times V_t)_{\mathsf{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

Cone of moment measures

- Define the operator $A_t \colon \mathcal{C}(V_t \times V_t)_{\mathsf{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

- A_t is a generalization of the dual of the operator that maps a vector to its moment matrix

Cone of moment measures

- Define the operator $A_t \colon \mathcal{C}(V_t \times V_t)_{\text{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

- A_t is a generalization of the dual of the operator that maps a vector to its moment matrix
- Cone of positive kernels: $\mathcal{C}(V_t \times V_t)_{\succeq 0}$

Cone of moment measures

- Define the operator $A_t\colon \mathcal{C}(V_t \times V_t)_{\mathrm{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

- A_t is a generalization of the dual of the operator that maps a vector to its moment matrix
- Cone of positive kernels: $\mathcal{C}(V_t \times V_t)_{\succeq 0}$
- Cone of moment measures

$$K_t(G) = \{\lambda \in \mathcal{M}(I_{\min\{2t,N\}})_{\geq 0} : A_t^* \lambda \in \mathcal{M}(V_t \times V_t)_{\succeq 0}\}$$

Cone of moment measures

- Define the operator $A_t \colon \mathcal{C}(V_t \times V_t)_{\mathsf{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

- A_t is a generalization of the dual of the operator that maps a vector to its moment matrix
- Cone of positive kernels: $\mathcal{C}(V_t \times V_t)_{\succeq 0}$
- Cone of moment measures

$$K_t(G) = \{\lambda \in \mathcal{M}(I_{\min\{2t,N\}})_{\geq 0} : A_t^* \lambda \in \mathcal{M}(V_t \times V_t)_{\succeq 0}\}$$

- When $t = N$, the extreme rays of $K_t(G)$ are precisely the measures χ_S with $S \in I_{=N}$

Cone of moment measures

- Define the operator $A_t \colon \mathcal{C}(V_t \times V_t)_{\text{sym}} \to \mathcal{C}(I_{\min\{2t,N\}})$ by

$$A_t K(S) = \sum_{J,J' \in V_t : J \cup J' = S} K(J, J')$$

- A_t is a generalization of the dual of the operator that maps a vector to its moment matrix
- Cone of positive kernels: $\mathcal{C}(V_t \times V_t)_{\succeq 0}$
- Cone of moment measures

$$K_t(G) = \{\lambda \in \mathcal{M}(I_{\min\{2t,N\}})_{\geq 0} : A_t^* \lambda \in \mathcal{M}(V_t \times V_t)_{\succeq 0}\}$$

- When $t = N$, the extreme rays of $K_t(G)$ are precisely the measures χ_S with $S \in I_{=N}$
- This is the main step in proving $E_N = E$

Dual hierarchy

- For lower bounds we need dual feasible solutions

Dual hierarchy

- For lower bounds we need dual feasible solutions
- In the dual hierarchy optimization is over scalars a_i and elements L in the dual cone $K_t(G)^*$

Dual hierarchy

- For lower bounds we need dual feasible solutions
- In the dual hierarchy optimization is over scalars a_i and elements L in the dual cone $K_t(G)^*$

$$E_t^* = \sup \Big\{ \sum_{i=0}^{\min\{2t,N\}} \binom{N}{i} a_i : \ a_0, \ldots, a_{\min\{2t,N\}} \in \mathbb{R},\ L \in K_t(G)^*, \\ a_i - L \leq w \ \text{ on } \ I_{=i} \ \text{ for } \ i = 0, \ldots, \min\{2t, N\} \Big\}$$

Dual hierarchy

- For lower bounds we need dual feasible solutions
- In the dual hierarchy optimization is over scalars a_i and elements L in the dual cone $K_t(G)^*$

$$E_t^* = \sup\Bigg\{ \sum_{i=0}^{\min\{2t,N\}} \binom{N}{i} a_i : \; a_0, \ldots, a_{\min\{2t,N\}} \in \mathbb{R},\; L \in K_t(G)^*,$$
$$a_i - L \leq w \;\text{ on }\; I_{=i} \;\text{ for }\; i = 0, \ldots, \min\{2t, N\} \Bigg\}$$

- The elements L are of the form $A_t K$ for $K \in \mathcal{C}(V_t \times V_t)_{\succeq 0}$

Dual hierarchy

- For lower bounds we need dual feasible solutions
- In the dual hierarchy optimization is over scalars a_i and elements L in the dual cone $K_t(G)^*$

$$E_t^* = \sup\left\{ \sum_{i=0}^{\min\{2t,N\}} \binom{N}{i} a_i : \; a_0, \ldots, a_{\min\{2t,N\}} \in \mathbb{R},\; L \in K_t(G)^*, \; a_i - L \leq w \;\text{ on }\; I_{=i} \;\text{ for }\; i = 0, \ldots, \min\{2t, N\} \right\}$$

- The elements L are of the form $A_t K$ for $K \in \mathcal{C}(V_t \times V_t)_{\succeq 0}$
- Strong duality holds: $E_t = E_t^*$

Frequency formulation

- Assume w is Γ-invariant: $w(\gamma x, \gamma y) = w(x, y)$ for all $\gamma \in \Gamma$, $x, y \in V$

Frequency formulation

- Assume w is Γ-invariant: $w(\gamma x, \gamma y) = w(x, y)$ for all $\gamma \in \Gamma$, $x, y \in V$
- Then all constraints in the program E_t^* are invariant under Γ, and we can restrict to the cone

$$\{A_t K : K \in \mathcal{C}(V_t \times V_t)^{\Gamma}_{\succeq 0}\}$$

Frequency formulation

- Assume w is Γ-invariant: $w(\gamma x, \gamma y) = w(x, y)$ for all $\gamma \in \Gamma$, $x, y \in V$
- Then all constraints in the program E_t^* are invariant under Γ, and we can restrict to the cone

$$\{A_t K : K \in \mathcal{C}(V_t \times V_t)^{\Gamma}_{\succeq 0}\}$$

- Γ acts on V_t by $\gamma\emptyset = \emptyset$ and $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$

Frequency formulation

- Assume w is Γ-invariant: $w(\gamma x, \gamma y) = w(x, y)$ for all $\gamma \in \Gamma$, $x, y \in V$
- Then all constraints in the program E_t^* are invariant under Γ, and we can restrict to the cone

$$\{A_t K : K \in \mathcal{C}(V_t \times V_t)_{\succeq 0}^{\Gamma}\}$$

- Γ acts on V_t by $\gamma\emptyset = \emptyset$ and $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$
- Bochner's theorem: $K \in \mathcal{C}(V_t \times V_t)_{\succeq 0}^{\Gamma}$ is of the form

$$K(J, J') = \sum_{k=0}^{\infty} \langle F_k, Z_k(J, J') \rangle \quad \text{where}$$

F_k: positive semidefinite matrices (the Fourier coefficients)
Z_k: zonal matrices corresponding to the action of Γ on V_t

Semidefinite programming

- Restrict the series $\sum_{k=0}^{\infty}\langle F_k, Z_k(J, J')\rangle$ to the first d terms

Semidefinite programming

- Restrict the series $\sum_{k=0}^{\infty} \langle F_k, Z_k(J, J') \rangle$ to the first d terms
- Use principal submatrices $Z_{k,d}$ of Z_k of size $s_{k,d}$
  (where $s_{k,d} \to \infty$ as $d \to \infty$)

Semidefinite programming

- Restrict the series $\sum_{k=0}^{\infty} \langle F_k, Z_k(J, J') \rangle$ to the first d terms
- Use principal submatrices $Z_{k,d}$ of Z_k of size $s_{k,d}$ (where $s_{k,d} \to \infty$ as $d \to \infty$)
- This gives a semi-infinite semidefinite program $E^*_{t,d}$

Semidefinite programming

- Restrict the series $\sum_{k=0}^{\infty}\langle F_k, Z_k(J, J')\rangle$ to the first d terms
- Use principal submatrices $Z_{k,d}$ of Z_k of size $s_{k,d}$ (where $s_{k,d} \to \infty$ as $d \to \infty$)
- This gives a semi-infinite semidefinite program $E^*_{t,d}$
- In general the Fourier series does not converge uniformly; the action of Γ on V_t has infinitely many orbits (for $t \geq 2$)

Semidefinite programming

- Restrict the series $\sum_{k=0}^{\infty}\langle F_k, Z_k(J, J')\rangle$ to the first d terms
- Use principal submatrices $Z_{k,d}$ of Z_k of size $s_{k,d}$ (where $s_{k,d} \to \infty$ as $d \to \infty$)
- This gives a semi-infinite semidefinite program $E^*_{t,d}$
- In general the Fourier series does not converge uniformly; the action of Γ on V_t has infinitely many orbits (for $t \geq 2$)
- By a summability method we have $E^*_{t,d} \to E^*_t$ as $d \to \infty$

Semidefinite programming

- The linear constraints in $E^*_{t,d}$ are of the form

$$a_i - \sum_{k=0}^{d} \langle F_k, A_t Z_{k,d} \rangle \leq w \ \text{ on } \ I_{=i} \ \text{ for } \ i = 0, \ldots, \min\{2t, N\}$$

Semidefinite programming

- The linear constraints in $E^*_{t,d}$ are of the form

$$a_i - \sum_{k=0}^{d} \langle F_k, A_t Z_{k,d} \rangle \leq w \ \text{ on } \ I_{=i} \ \text{ for } \ i = 0, \ldots, \min\{2t, N\}$$

- Variable transformation to write the above as polynomial inequalities over a semialgebraic set (depends on the application)

Semidefinite programming

- The linear constraints in $E_{t,d}^*$ are of the form

$$a_i - \sum_{k=0}^{d} \langle F_k, A_t Z_{k,d} \rangle \leq w \text{ on } I_{=i} \text{ for } i = 0, \ldots, \min\{2t, N\}$$

- Variable transformation to write the above as polynomial inequalities over a semialgebraic set (depends on the application)
- Using sums of squares characterizations $E_{t,d}^*$ can be approximated by a sequence of finite semidefinite programs

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- Zonal matrices as polynomial matrices in the inner products:

$$Z_k(\{x_1, \ldots, x_t\}, \{y_1, \ldots, y_t\})_{i,j} = \left(\prod_{r,s=1}^{t} (x_r \cdot x_s)^i (y_r \cdot y_s)^j \right) \sum_{r,s=1}^{t} T_k(x_r \cdot y_s)$$

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- Zonal matrices as polynomial matrices in the inner products:

$$Z_k(\{x_1,\ldots,x_t\},\{y_1,\ldots,y_t\})_{i,j} = \left(\prod_{r,s=1}^{t} (x_r \cdot x_s)^i (y_r \cdot y_s)^j\right) \sum_{r,s=1}^{t} T_k(x_r \cdot y_s)$$

- $A_t Z_{k,d}$ is an $O(2)$-invariant matrix valued function on sets in $I_{\min\{2t,N\}}$

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- Zonal matrices as polynomial matrices in the inner products:

$$Z_k(\{x_1,\ldots,x_t\},\{y_1,\ldots,y_t\})_{i,j} = \left(\prod_{r,s=1}^{t}(x_r\cdot x_s)^i(y_r\cdot y_s)^j\right)\sum_{r,s=1}^{t} T_k(x_r\cdot y_s)$$

- $A_t Z_{k,d}$ is an $O(2)$-invariant matrix valued function on sets in $I_{\min\{2t,N\}}$
- Describe an element $\{x_1,\ldots,x_{\min\{2t,N\}}\} \in (I_{\min\{2t,N\}})/O(2)$ by the angles $\theta_i = \cos(x_i\cdot x_{i+1})$ for $i = 1,\ldots,\min\{2t,N\}-1$

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- Zonal matrices as polynomial matrices in the inner products:

$$Z_k(\{x_1,\ldots,x_t\},\{y_1,\ldots,y_t\})_{i,j} = \left(\prod_{r,s=1}^{t}(x_r\cdot x_s)^i(y_r\cdot y_s)^j\right)\sum_{r,s=1}^{t}T_k(x_r\cdot y_s)$$

- $A_t Z_{k,d}$ is an $O(2)$-invariant matrix valued function on sets in $I_{\min\{2t,N\}}$
- Describe an element $\{x_1,\ldots,x_{\min\{2t,N\}}\} \in (I_{\min\{2t,N\}})/O(2)$ by the angles $\theta_i = \cos(x_i\cdot x_{i+1})$ for $i = 1,\ldots,\min\{2t,N\}-1$
- Each inner product is a trigonometric polynomial in these angles

Example: $V = S^1$ with $O(2)$-invariant pair potential w

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- The linear inequalities should hold over the set

$$\left\{(\theta_1, \ldots, \theta_{\min\{2t,N\}}) : \cos\left(\sum_{i \in E} \theta_i\right) \geq C_\delta \text{ for } E \subseteq \{1, \ldots, \min\{2t, N\}\}\right\}$$

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- The linear inequalities should hold over the set

$$\left\{(\theta_1, \dots, \theta_{\min\{2t,N\}}) : \cos\left(\sum_{i \in E} \theta_i\right) \geq C_\delta \text{ for } E \subseteq \{1, \dots, \min\{2t, N\}\}\right\}$$

- Use trigonometric SOS characterizations [Dumitrescu 2006]

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- The linear inequalities should hold over the set

$$\left\{(\theta_1, \ldots, \theta_{\min\{2t,N\}}) : \cos\left(\sum_{i \in E} \theta_i\right) \geq C_\delta \text{ for } E \subseteq \{1, \ldots, \min\{2t, N\}\}\right\}$$

- Use trigonometric SOS characterizations [Dumitrescu 2006]
- The 4-point bound E_2^* requires trivariate SOS characterizations

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- The linear inequalities should hold over the set

$$\left\{(\theta_1, \ldots, \theta_{\min\{2t,N\}}) : \cos\left(\sum_{i \in E} \theta_i\right) \geq C_\delta \text{ for } E \subseteq \{1, \ldots, \min\{2t, N\}\}\right\}$$

- Use trigonometric SOS characterizations [Dumitrescu 2006]
- The 4-point bound E_2^* requires trivariate SOS characterizations
- For Coulomb (or other completely monotonic potentials) 2-point bounds are always sharp on the circle Cohn-Kumar 2006

Example: $V = S^1$ with $O(2)$-invariant pair potential w

- The linear inequalities should hold over the set

$$\left\{(\theta_1, \ldots, \theta_{\min\{2t,N\}}) : \cos\left(\sum_{i \in E} \theta_i\right) \geq C_\delta \text{ for } E \subseteq \{1, \ldots, \min\{2t, N\}\}\right\}$$

- Use trigonometric SOS characterizations [Dumitrescu 2006]
- The 4-point bound E_2^* requires trivariate SOS characterizations
- For Coulomb (or other completely monotonic potentials) 2-point bounds are always sharp on the circle Cohn-Kumar 2006
- Lennard-Jones potential: Based on a sampling implementation it appears that for e.g. $N = 3$ we have

$$E_1 < E_2 = E$$

Thank you!