Energy minimization via conic programming hierarchies

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- Optimization problem:

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

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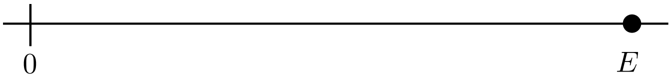
- For this we use infinite dimensional moment hierarchies and semidefinite programming

Approach



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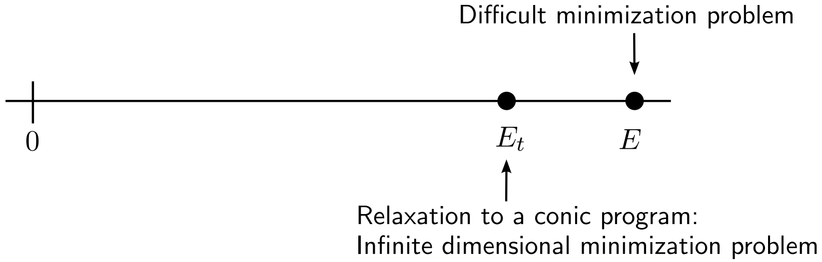
Difficult minimization problem
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Infinite dimensional minimization problem

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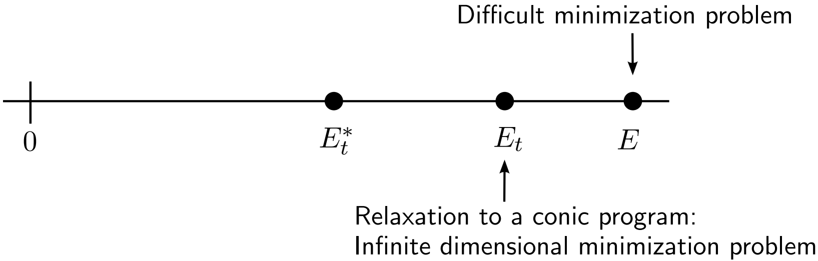
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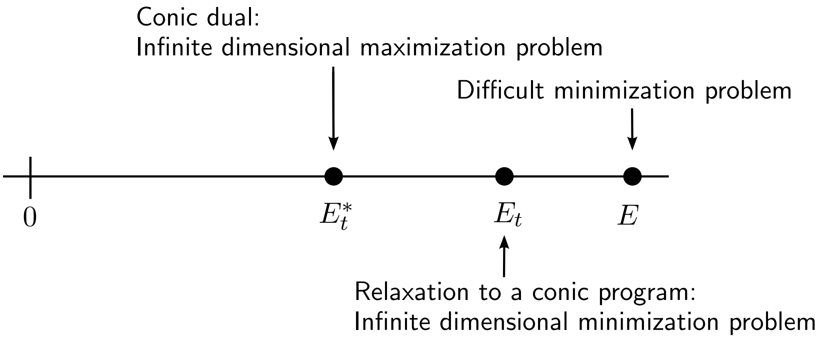
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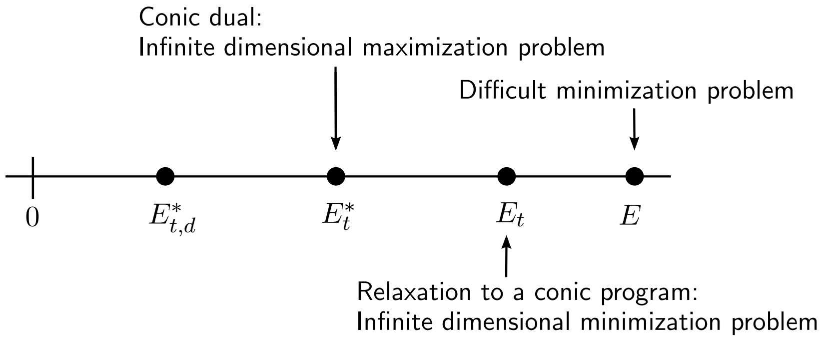
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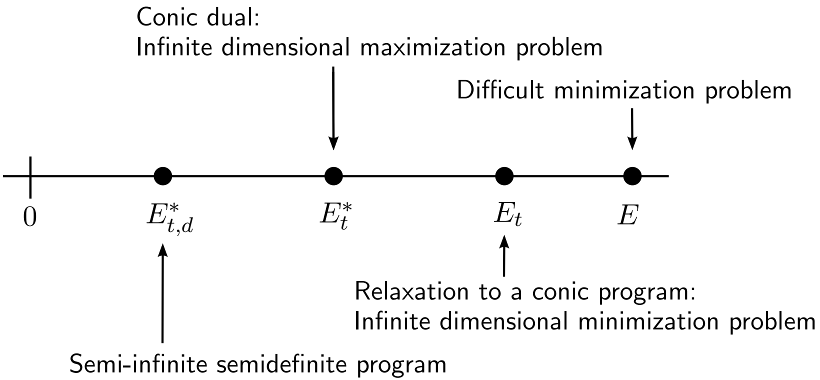
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Semi-infinite semidefinite program

Finite container

- If $V = \{1, \ldots, n\}$ is a finite set, then E is a polynomial optimization problem:

$$E = \min \left\{ \sum_{\{i,j\} \in \binom{V}{2}} w(\{i,j\}) x_i x_j : x \in \{0,1\}^n, \sum_{i \in V} x_i = N \right\}$$

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- The Lasserre hierarchy gives a chain $E_1 \leq E_2 \leq \cdots \leq E_n$ of lower bounds to the optimal energy E:

$$E_t = \min \Bigg\{ \sum_{S \in \binom{V}{2}} w(S) y(S) : y \in \mathbb{R}^{\binom{V}{\leq 2t}},\ y(\emptyset) = 1,\ \big(y(A \cup B)\big)_{A,B \in \binom{V}{\leq t}} \succeq 0,$$
$$\sum_{x \in V} y(T \cup \{x\}) = N y(T) \text{ for } T \in \binom{V}{\leq 2t-1} \Bigg\}$$

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- Uses techniques from [de Laat-Vallentin 2013]: hierarchy for packing problems in discrete geometry

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- If Γ acts on V and w is Γ-invariant, then we can restrict to Γ-invariant kernels: $K(\gamma J, \gamma J') = K(J, J')$ for all $J, J' \in \binom{V}{\le t}$ (Here $\gamma\{x_1, \ldots, x_t\} = \{\gamma x_1, \ldots, \gamma x_t\}$)

Inner approximiations to the cone $\mathcal{C}(\binom{V}{\leq t} \times \binom{V}{\leq t})^{\Gamma}_{\succeq 0}$

- Nested chain of inner approximations:

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$$K(J, J') = \sum_{k=0}^{\infty} \operatorname{trace}(F_k Z_k(J, J'))$$

  - F_k: (infinite) positive semidefinite matrices (the Fourier coefficients)
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- Define C_d by truncating the above series

The semi-infinite semidefinite programs $E^*_{t,d}$

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- This is an optimization problem with finitely many variables and infinitely many constraints
- $E_{t,d}^* \to E_t^*$ as $d \to \infty$ follows from $\cup_{d=0}^{\infty} C_d$ being uniformly dense in $\mathcal{C}(\binom{V}{\leq t} \times \binom{V}{\leq t})_{\succeq 0}^{\Gamma}$

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- The bound E^*_2 requires SOS characterizations in 3 variables
- 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!