Mathematics > Optimization and Control

Canonical dual theory applied to a Lennard-Jones potential minimization problem

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The simplified Lennard-Jones (LJ) potential minimization problem is $f(x)=4\sum_{i=1}^N \sum_{j=1,j<i}^N (\frac{1}{\tau_{ij}^6} -\frac{1}{\tau_{ij}^3}) {subject to} x\in \mathbb{R}^n,$ where $\tau_{ij}=(x_{3i-2}-x_{3j-2})^2 +(x_{3i-1}-x_{3j-1})^2 +(x_{3i} -x_{3j})^2$, $(x_{3i-2},x_{3i-1},x_{3i})$ is the coordinates of atom i in $\mathbb{R}^3$, $i,j=1,2,...,N(\geq 2 \quad \text{integer})$, $n=3N$ and N is the whole number of atoms. The nonconvexity of the objective function and the huge number of local minima, which is growing exponentially with N, interest many mathematical optimization experts. In this paper, the canonical dual theory elegantly tackles this problem illuminated by the amyloid fibril molecular model building.
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