GLOBAL OPTIMAL SOLUTIONS TO NONCONVEX EUCLIDEAN DISTANCE GEOMETRY PROBLEMS

NING RUAN* AND DAVID YANG GAO†

Abstract. This paper presents a canonical dual approach for solving nonconvex minimization problems in Euclidean distance geometry. The variant of this problem arises extensively in engineering and science, including computational biology, sensor network communications, database analysis, information technology, and global optimization. Due to the nonconvexity, most of these problems are NP-hard and traditional convex optimization methods can not be used directly for finding global optimal solutions. We first show that this type of nonconvex problems can be transferred to a concave maximization problem over a convex set. Then a general analytical solution is proposed by using the canonical duality theory. Applications are illustrated by network localization and minimization of Rosenbrock function. Furthermore, by using a perturbed canonical dual approach, a class of Euclidean distance problems can be converted to a unified concave maximization dual problem with zero duality gap, which can be solved by well-developed convex minimization methods.

Key words. duality theory, nonconvex programming, global optimization, database analysis, canonical duality theory

AMS subject classifications. 90C22,90C25,90C26

1. Introduction.

We are interested in solving the following general nonlinear programming problem arising from Euclidean distance geometry (see [4]):

$$(\mathcal{P}) \quad \min \left\{ P(\mathbf{X}) = \sum_{(i,j)\in\mathcal{S}} \frac{1}{2} w_{ij} \left(\frac{1}{2}\|\mathbf{x}_i - \mathbf{x}_j\|^2 - \mu_{ij} \right)^2 + \frac{1}{2}\langle \mathbf{X}, \mathbf{A}\mathbf{X}\rangle - \langle \mathbf{X}, \mathbf{T}\rangle \ | \ \mathbf{X} \in \mathcal{X}_a \right\},$$

where the decision variable $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n] = \{x_i^\alpha\}_{i,\alpha} \in \mathbb{R}^{r\times n}$ is a matrix (two-point tensor) with each column $\mathbf{x}_i \in \mathbb{R}^r$ as a position of each sensor such that

$$\|\mathbf{x}_i - \mathbf{x}_j\| = \sqrt{\sum_{\alpha=1}^{r} (x_i^\alpha - x_j^\alpha)^2}$$

denotes the Euclidian distance between $\mathbf{x}_i$ and $\mathbf{x}_j$, $(i,j) \in \mathcal{S} = \{1,2,\cdots,n\}$; $\mathcal{X}_a \subset \mathbb{R}^{d\times n}$ is a feasible set; $\mathbf{T} = \{T_\alpha^i\} \in \mathcal{X}^* = \mathbb{R}^{n\times d}$ is a given matrix; $w_{ij} \geq 0$ and $\mu_{ij} \geq 0$ $(\forall i,j \in \mathcal{S})$ are given weights and parameters for each pair $(\mathbf{x}_i, \mathbf{x}_j)$, respectively; $\mathbf{A} = \{A_{\alpha,j}^{i,\beta}\}$ is a fourth-order symmetric tensor, satisfying

$$A_{\alpha,j}^{i,\beta} = A_{\beta,j}^{i,\alpha} = A_{\alpha,i}^{j,\beta} \quad \forall \alpha,\beta = 1,\cdots,d, \ \ i,j = 1,\cdots,n.$$

In this paper, the product $\mathbf{AX}$ is understood as

$$\mathbf{AX} = \{\sum_{j=1}^{n}\sum_{\beta=1}^{r} \mathbf{A}_{\alpha,j}^{i,\beta} x_j^\beta\}_{i,\alpha},$$

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the bilinear form $\langle \mathbf{X}, \mathbf{T}\rangle : \mathcal{X}_a \times \mathcal{X}^* \to \mathbb{R}$ is defined as

$$\langle \mathbf{X}, \mathbf{T}\rangle = tr(\mathbf{X}\mathbf{T}) = \sum_{i=1}^{n}\sum_{\alpha=1}^{d} X_i^\alpha T_\alpha^i.$$

The distance geometry problem [12, 15] can also be viewed as a variant of sensor network localization problem or a graph realization problem which has been studied extensively in computational biology, Euclidean ball packing, pharmaceutical, and recently, wireless network communication. For example, molecular conformation which using inter-atomic distance information has an extremely important application in biology for protein structure prediction and determination [1, 8]. In general, the distance geometry problem is considered to be NP-hard even for the simplest case $r = 1$ [11, 14]. Therefore, many approximation methods have been proposed for solving this nonconvex, nonsmooth global optimization problem. The semi-definite programming (SDP) and second-order cone programming (SOCP) relaxations are two of the popular methods studied recently [1, 2, 3, 16, 17]. Similar to the linear primal-dual interior point methods, many numerical schemes for SDP or SOCP often return to the analytic center of the solution set.

In order to solve a variety of nonconvex variational problems, a unified *canonical duality theory* has been developed from nonlinear analysis of finite deformation theory and finite element analysis of large scale computational mechanics, which leads to a general analytical solution form. It is now realized that this canonical duality theory is potentially powerful for solving a large class of challenging problems in global optimization. The purpose of this paper is to demonstrate the potentials of the canonical duality theory by solving the proposed primal problem $(\mathcal{P})$.

2. Main results.

2.1. Canonical geometric measure and dual problem. Since

$$\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n) \in \mathbb{R}^{r\times n},$$

we have the identity

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2 = (\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j) = (\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{X}^T \mathbf{X}(\mathbf{e}_i - \mathbf{e}_j),$$

where $\mathbf{e}_i$ is the i-th standard unit vector in $\mathbb{R}^n$. Introducing a linear (difference) operator $\mathbf{D} : \mathcal{X}_a \to \mathbb{R}^{r\times n\times n}$ such that

$$\mathbf{D}\mathbf{X} = \{\mathbf{X}(\mathbf{e}_i - \mathbf{e}_j)\} = \{\mathbf{x}_i - \mathbf{x}_j\},$$

the *canonical strain measure* $\boldsymbol{\xi}$ can be defined as

$$\boldsymbol{\xi} = \{\boldsymbol{\xi}_{ij}\}_{i,j} = \Lambda(\mathbf{X}) = \frac{1}{2}(\mathbf{D}\mathbf{X})^T(\mathbf{D}\mathbf{X}) = \frac{1}{2}\left\{(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{X}^T \mathbf{X}(\mathbf{e}_i - \mathbf{e}_j)\right\},$$

where Λ is the so-called *geometrical nonlinear operator* from $\mathcal{X}_a \subset \mathbb{R}^{r\times n}$ into $\mathcal{V}_a = \{\boldsymbol{\varepsilon} \in \mathbb{R}^{n\times n} |\ \boldsymbol{\xi} = \boldsymbol{\xi}^T,\ \boldsymbol{\xi} \succeq 0,\ \xi_{ii} = 0,\ i = 1, \cdots, n\}$. Clearly, $\xi_{ij} = \frac{1}{2}\|\mathbf{x}_i - \mathbf{x}_j\|^2$, which is corresponding to the Cauchy-Riemann strain tensor in finite deformation theory. By introducing a quadratic function $V : \mathcal{V}_a \to \mathbb{R}$,

$$V(\boldsymbol{\xi}) = \frac{1}{2}\sum_{i,j} w_{ij}(\xi_{ij} - \mu_{ij})^2 = \frac{1}{2}\langle(\boldsymbol{\xi} - \boldsymbol{\mu}); \mathbf{W} \circ (\boldsymbol{\xi} - \boldsymbol{\mu})\rangle,$$

where $\mathbf{W} = \{w_{ij}\}$, $\boldsymbol{\mu} = \{\mu_{ij}\}$, $\mathbf{W} \circ \boldsymbol{\mu} = \{w_{ij}\mu_{ij}\}$ represents the Hadamard product of two matrices, and $\langle ; \rangle$ denotes the bilinear operator of two matrices. The primal problem $(\mathcal{P})$ can now be reformulated in the canonical form as follows:

$$(\mathcal{P}): \quad \min \left\{ \Pi(\mathbf{X}) = V(\Lambda(\mathbf{X})) + \frac{1}{2}\langle \mathbf{X}, \mathbf{A}\mathbf{X} \rangle - \langle \mathbf{X}, \mathbf{T} \rangle : \quad \mathbf{X} \in \mathcal{X}_a \right\}.$$

By the fact that the function $V(\boldsymbol{\xi})$ is convex, the duality relation

$$\boldsymbol{\varsigma} = \delta V(\boldsymbol{\xi}) = \mathbf{W} \circ (\boldsymbol{\xi} - \boldsymbol{\mu})$$

is invertible for any given $\boldsymbol{\xi} \in \mathcal{V}_a$. Let $\mathcal{V}_a^*$ be the range of the duality mapping $\boldsymbol{\varsigma} = \delta V(\boldsymbol{\xi}) : \mathcal{V}_a \to \mathcal{V}_a^* \subset \mathbb{R}^{n\times n}$ and let

$$\langle \boldsymbol{\xi}; \boldsymbol{\varsigma} \rangle = \sum_{i,j \in \mathcal{S}} \xi_{ij} \varsigma_{ij}$$

denote a bilinear form on $\mathcal{V} \times \mathcal{V}^*$. Thus, for any given $\boldsymbol{\varsigma} \in \mathcal{V}_a^*$, the Legendre conjugate V^* can be uniquely defined by

$$V^*(\boldsymbol{\varsigma}) = \text{sta}\{\langle \boldsymbol{\xi}; \boldsymbol{\varsigma} \rangle - V(\boldsymbol{\varepsilon}) \mid \boldsymbol{\varepsilon} \in \mathcal{V}_a\} = \frac{1}{2}\langle \boldsymbol{\varsigma}; \mathbf{W}^{-1} \circ \boldsymbol{\varsigma} \rangle + \langle \boldsymbol{\mu}; \boldsymbol{\varsigma} \rangle,$$

where sta{} denotes finding the stationary point of the statement in {}. So $(\boldsymbol{\xi}; \boldsymbol{\varsigma})$ forms a *canonical duality pair* on $\mathcal{V}_a \times \mathcal{V}_a^*$ (cf. [5]) and the following canonical duality relations hold on $\mathcal{V}_a \times \mathcal{V}_a^*$:

$$\boldsymbol{\varsigma} = \delta V(\boldsymbol{\varepsilon}) \quad \Leftrightarrow \quad \boldsymbol{\varepsilon} = \delta V^*(\boldsymbol{\varsigma}) \quad \Leftrightarrow \quad \langle \boldsymbol{\varepsilon}; \boldsymbol{\varsigma} \rangle = V(\boldsymbol{\varepsilon}) + V^*(\boldsymbol{\varsigma}).$$

Replacing $V(\Lambda(\mathbf{X}))$ by $\langle \Lambda(\mathbf{X}); \boldsymbol{\varsigma} \rangle - V^*(\boldsymbol{\varsigma})$, the generalized complementary function ([5]) can be defined by

$$\begin{aligned} \Xi(\mathbf{X}, \boldsymbol{\varsigma}) &= \langle \frac{1}{2}(\mathbf{D}\mathbf{X})^T(\mathbf{D}\mathbf{X}); \boldsymbol{\varsigma} \rangle - V^*(\boldsymbol{\varsigma}) + \frac{1}{2}\langle \mathbf{X}, \mathbf{A}\mathbf{X} \rangle - \langle \mathbf{X}, \mathbf{T} \rangle \\ &= \frac{1}{2}\langle \mathbf{X}, \mathbf{G}(\boldsymbol{\varsigma})\mathbf{X} \rangle - V^*(\boldsymbol{\varsigma}) - \langle \mathbf{X}, \mathbf{T} \rangle, \end{aligned}$$

where $\mathbf{G}(\boldsymbol{\varsigma}) = \mathbf{A} + \mathbf{D}^T \boldsymbol{\varsigma} \mathbf{D}$ and $\mathbf{D}^T \boldsymbol{\varsigma} = (\mathbf{e}_i^T - \mathbf{e}_j^T)\boldsymbol{\varsigma}$. For a fixed $\boldsymbol{\varsigma} \in \mathcal{V}_a^*$, the criticality condition $\delta_{\mathbf{X}} \Xi(\mathbf{X}, \boldsymbol{\varsigma}) = 0$ leads to the following *canonical equilibrium equation*:

$$\mathbf{G}(\boldsymbol{\varsigma})\mathbf{X} - \mathbf{T} = 0,$$

Thus, on the dual feasible space defined by $\mathcal{S}_a \subset \mathbb{R}^{n\times n}$, the canonical dual function can be formulated as

$$P^d(\boldsymbol{\varsigma}) = \text{sta}\{\Xi(\mathbf{X}, \boldsymbol{\varsigma}) : \ \mathbf{X} \in \mathcal{X}_a\} = -\frac{1}{2}\langle \mathbf{G}^+(\boldsymbol{\varsigma})\mathbf{T}, \mathbf{T} \rangle - V^*(\boldsymbol{\varsigma}).$$

Thus, the canonical dual problem can be proposed as follows:

$$(\mathcal{P}^d): \quad \text{sta} \left\{ P^d(\boldsymbol{\varsigma}) = -\frac{1}{2}\langle \mathbf{G}^+(\boldsymbol{\varsigma})\mathbf{T}, \mathbf{T} \rangle - \frac{1}{2}\langle \boldsymbol{\varsigma}; \mathbf{W}^{-1} \circ \boldsymbol{\varsigma} \rangle - \langle \boldsymbol{\mu}; \boldsymbol{\varsigma} \rangle \ \mid \ \boldsymbol{\varsigma} \in \mathcal{S}_a \right\}.$$

THEOREM 2.1 (Complementary-Dual Principle). *The problem $(\mathcal{P}^d)$ is a canonical dual of the primal problem $(\mathcal{P})$ in the sense that if $\bar{\boldsymbol{\varsigma}}$ is a critical point of $(\mathcal{P}^d)$, then*

$$\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\boldsymbol{\varsigma}})\mathbf{T} \tag{2.1}$$

is a critical point of $(\mathcal{P})$ *and*

$$P(\bar{\mathbf{X}}) = P^d(\bar{\varsigma}).$$

Proof. Suppose that $\bar{\varsigma}$ is a critical point of $(\mathcal{P}^d)$. Then, we have

$$\nabla P^d(\bar{\varsigma}) = \frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \mathbf{W}^{-1}\bar{\varsigma} - \boldsymbol{\mu} = 0,$$

where $\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T}$. The criticality condition (2.2) is actually the canonical duality relation (constitutive equation), i.e., $\varsigma = \mathbf{W} \circ (\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \boldsymbol{\mu})$. Thus, we have

$$\begin{aligned}\bar{\mathbf{X}} &= \mathbf{G}^+(\bar{\varsigma})\mathbf{T} \\ &= \left[\mathbf{A} + \mathbf{D}^T(\mathbf{W} \circ (\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \boldsymbol{\mu})\mathbf{D}\right]^+ \mathbf{T}.\end{aligned}$$

This shows that $\bar{\mathbf{X}}$ is a critical point of the primal problem $(\mathcal{P})$.

Moreover, in term of $\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T}$, we have

$$\begin{aligned}P^d(\bar{\varsigma}) &= -\frac{1}{2}\langle(\mathbf{A} + \mathbf{D}^T\bar{\varsigma}\mathbf{D})^+\mathbf{T}, \mathbf{T}\rangle - \frac{1}{2}\langle\bar{\varsigma}; \mathbf{W}^{-1} \circ \bar{\varsigma}\rangle - \langle\boldsymbol{\mu}; \bar{\varsigma}\rangle \\ &= \frac{1}{2}\langle(\mathbf{A} + \mathbf{D}^T\bar{\varsigma}\mathbf{D})^+\mathbf{T}, \mathbf{T}\rangle - \langle\bar{\mathbf{X}}, \mathbf{T}\rangle - \frac{1}{2}\langle\bar{\varsigma}; \mathbf{W}^{-1} \circ \bar{\varsigma}\rangle - \langle\boldsymbol{\mu}; \bar{\varsigma}\rangle \\ &= \frac{1}{2}\langle\bar{\mathbf{X}}, (\mathbf{A} + \mathbf{D}^T\bar{\varsigma}\mathbf{D})\bar{\mathbf{X}}\rangle - \langle\bar{\mathbf{X}}, \mathbf{T}\rangle - \frac{1}{2}\langle\bar{\varsigma}; \mathbf{W}^{-1} \circ \bar{\varsigma}\rangle - \langle\boldsymbol{\mu}; \bar{\varsigma}\rangle \\ &= \frac{1}{2}\langle\bar{\mathbf{X}}, \mathbf{A}\bar{\mathbf{X}}\rangle - \langle\bar{\mathbf{X}}, \mathbf{T}\rangle + \langle\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}); \bar{\varsigma}\rangle - \frac{1}{2}\langle\bar{\varsigma}; \mathbf{W}^{-1} \circ \bar{\varsigma}\rangle - \langle\boldsymbol{\mu}; \bar{\varsigma}\rangle \\ &= \frac{1}{2}\langle\bar{\mathbf{X}}, \mathbf{A}\bar{\mathbf{X}}\rangle - \langle\bar{\mathbf{X}}, \mathbf{T}\rangle + \frac{1}{2}\langle[\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \boldsymbol{\mu}]; \mathbf{W} \circ [\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \boldsymbol{\mu}]\rangle \\ &= P(\bar{\mathbf{X}}).\end{aligned}$$

This proves the theorem. □

In order to identify extremality properties of the analytical solution (2.1), we need to introduce this useful feasible space

$$\mathcal{S}_a^+ = \{\varsigma \in \mathcal{S}_a \mid \ \mathbf{G}(\varsigma) \succ 0\}.$$

THEOREM 2.2. *Suppose that* $\bar{\varsigma}$ *is a critical point of the canonical dual function* $P^d(\bar{\varsigma})$ *and* $\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T}$*. Let* $\bar{\varsigma} \in \mathcal{S}_a^+$*. Then,* $\bar{\mathbf{X}}$ *is a global minimizer of* $P(\mathbf{X})$ *on* $\mathbb{R}^{r\times n}$ *if and only if* $\bar{\varsigma}$ *is a global maximizer of* $P^d(\varsigma)$ *on* $\mathcal{S}_a^+$*, i.e.,*

$$P(\bar{\mathbf{X}}) = \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} P(\mathbf{X}) \Leftrightarrow \max_{\varsigma\in\mathcal{S}_a^+} P^d(\varsigma) = P^d(\bar{\varsigma}). \tag{2.2}$$

Proof. By Theorem 2.1 and the canonical duality theory [5], we know that vector $\bar{\varsigma} \in \mathcal{S}_a$ is a critical point of the problem $(\mathcal{P}^d)$ if and only if $\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T}$ is a critical point of the problem $(\mathcal{P})$, and

$$P(\bar{\mathbf{X}}) = \Xi(\bar{\mathbf{X}}, \bar{\varsigma}) = P^d(\bar{\varsigma}).$$

By the fact that the canonical dual function $P^d(\varsigma)$ is concave on $\mathcal{S}_a^+$, the critical point $\bar{\varsigma} \in \mathcal{S}_a^+$ is a global maximizer of $P^d(\varsigma)$ over $\mathcal{S}_a^+$. Since $(\bar{\mathbf{X}}, \bar{\varsigma})$ is a saddle point of the total complementary function $\Xi(\mathbf{X}, \boldsymbol{\varsigma})$ on $\mathbb{R}^{r\times n} \times \mathcal{S}_a^+$, i.e., Ξ is convex in $\mathbf{X} \in \mathbb{R}^{r\times n}$ and concave in $\boldsymbol{\varsigma} \in \mathcal{S}_a^+$, it follows from the canonical min-max duality theory (see[5]) that

$$\begin{aligned}
& P^d(\bar{\varsigma}) \\
&= \max_{\varsigma \in \mathcal{S}_a^+} P^d(\varsigma) = \max_{\varsigma \in \mathcal{S}_a^+} \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} \Xi(\mathbf{X}, \varsigma) = \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} \max_{\varsigma \in \mathcal{S}_a^+} \Xi(\mathbf{X}, \varsigma) \\
&= \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} \left\{ \frac{1}{2}\langle \mathbf{X}, \mathbf{A}\mathbf{X}\rangle - \langle \mathbf{X}, \mathbf{T}\rangle + \max_{\varsigma \in \mathcal{S}_a^+} \left\{ \langle \frac{1}{2}(\mathbf{D}\mathbf{X})^T(\mathbf{D}\mathbf{X}); \varsigma\rangle \right.\right. \\
&\qquad \left.\left. -(\frac{1}{2}\langle \varsigma; \mathbf{W}^+ \circ \varsigma\rangle + \langle \boldsymbol{\mu}; \varsigma\rangle) \right\}\right\} \\
&= \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} \left\{ \frac{1}{2}\langle \mathbf{X}, \mathbf{A}\mathbf{X}\rangle - \langle \mathbf{X}, \mathbf{T}\rangle + \frac{1}{2}\langle [\frac{1}{2}(\mathbf{D}\mathbf{X})^T(\mathbf{D}\mathbf{X}) - \boldsymbol{\mu}]; \mathbf{W} \circ [\frac{1}{2}(\mathbf{D}\mathbf{X})^T(\mathbf{D}\mathbf{X}) - \boldsymbol{\mu}]\rangle \right\} \\
&= \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} P(\mathbf{X}) = P(\bar{\mathbf{X}})
\end{aligned}$$

This proves the statement (2.2). □

2.2. Numerical experiments.

2.2.1. 18 sensors network localization problem. We now consider sensor network localization problem with 18 sensors. In this case, we have Problem $(\mathcal{P}_1)$ with $d = 2$. Define $\mathbf{y} = [x_1^1, x_1^2, \cdots, x_n^1, x_n^2]^T \in \mathbb{R}^{2n}$, and let $w_{ij} = q_{ik} = 1$ in Problem $(\mathcal{P}_1)$. Here, we do not consider noise.

The 18 sensors $\{\hat{\mathbf{x}}_i = [\hat{x}_i^1, \hat{x}_i^2] : i = 1, \cdots, 18\}$ are randomly generated in the unit square [-0.5, 0.5] × [-0.5, 0.5]. The four anchors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$ are placed at the positions $(\pm 0.45, \pm 0.45)$. The distances $\mathbf{d} = \{d_{ij}\}$, $i = 1, \cdots, 18$; $j = 1, \cdots, 18$, and $\mathbf{e} = \{e_{ik}\}$, $i = 1, \cdots, 18$; $k = 1, \cdots, 4$, are computed as follows:

$$d_{ij} = \|x_i^* - x_j^*\|, \; e_{ik} = \|x_i^* - a_k\|$$

We now assume that the locations of the 18 sensors are unknown. They are to be determined by the approach proposed in the paper. The sequential quadratic programming approximation with active set strategy in the optimization toolbox within the Matlab environment is used to solve the canonical dual problem.

By Theorem 2.2, we obtain $\bar{\mathbf{y}} = [\bar{\mathbf{x}}_1, \cdots, \bar{\mathbf{x}}_{18}]^T$ with $\bar{\mathbf{x}}_i = [\bar{\mathbf{x}}_i^1, \bar{\mathbf{x}}_i^2]^T, i = 1, \cdots, 18$, which is a global minimizer of $P(\mathbf{y})$,

Furthermore, we have

$$\Pi(\bar{\mathbf{y}}) = 1.30 \times 10^{-8} \simeq 3.03 \times 10^{-8} = \Pi^d(\bar{\boldsymbol{\varsigma}}, \bar{\boldsymbol{\sigma}}).$$

This problem is also solved by the standard semi-definite programming (SDP) method. The RMSD obtained using the canonical dual method is 4.61×10^{-7}, while the RMSD obtained using the standard SDP method is 4.45×10^{-5}, where RMSD is the Root Mean Square Distance defined by

$$\text{RMSD} = (\frac{1}{n}\sum_{i=1}^{n} \|\hat{\mathbf{x}}_i - \bar{\mathbf{x}}_i\|^2)^{\frac{1}{2}},$$

which is to measure the accuracy of the computed locations.

The computed results by the canonical dual method and the standard SDP method are plotted in Fig. 2.1 and Fig. 2.2, respectively. The true sensor locations

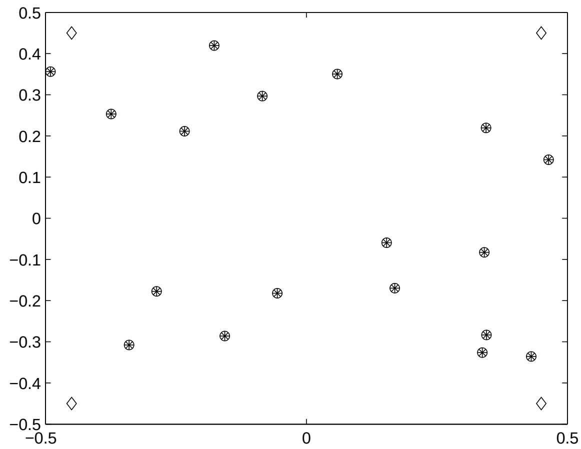

FIG. 2.1. *Sensor network with 18 sensors by the canonical dual method.*

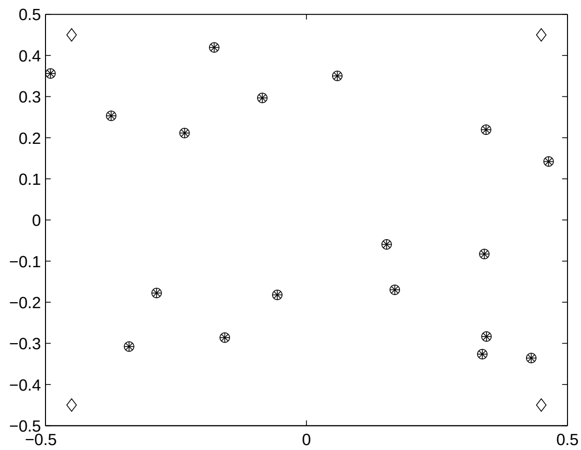

FIG. 2.2. *Sensor network with 18 sensors by the standard SDP method.*

(denoted by circles) and the computed locations (denoted by stars) are connected by solid lines. Our program is implemented in the MATLAB environment, where SEDUMI is used as the SDP solver.

From the results obtained, we see that, when there is no noise and the sensor size is not too large, both the canonical dual method and SDP method are very effective method for finding sensor locations. In particular, for the canonical dual method, all the stars are exactly located inside circles.

2.2.2. Minimization problem of Rosenbrock function.

$$(\mathcal{P}): \quad \min \left\{ P(x) = \sum_{i=1}^{n-1} \left[(x_i - 1)^2 + \frac{1}{2}\alpha(x_{i+1} - x_i^2)^2 \right] \; : \; x \in \mathcal{X} \right\}, \qquad (2.3)$$

where $x = \{x_i\} \in \mathcal{X} = \mathbb{R}^n$ is a real unknown vector, $\alpha = 2N$ and N is a given real number, say N=100. This is a well-known test problem for global optimization. Clearly, this is a nonconvex minimization problem which could have multiple local minimizers.

By introducing the canonical dual feasible space

$$\mathcal{S}_a = \{\boldsymbol{\varsigma} \in \mathbb{R}^{n-1} : \ \varsigma_i + 1 \neq 0 \ \ \forall i = 1, \ldots, n-2, \ \varsigma_{n-1} = 0\}, \tag{2.4}$$

and convex dual feasible space

$$\mathcal{S}_a^+ = \{\boldsymbol{\varsigma} \in \mathcal{S}_a : \ \varsigma_i + 1 > 0 \ \ \forall i = 1, \ldots, n-1\}, \tag{2.5}$$

the canonical dual problem can be specified as a concave maximization problem:

$$(\mathcal{P}^d) : \ \ \max\{P^d(\boldsymbol{\varsigma}) \ : \ \boldsymbol{\varsigma} \in \mathcal{S}_a^+\}. \tag{2.6}$$

where

$$P^d(\boldsymbol{\varsigma}) = \text{sta}\{\Xi(\mathbf{x}, \boldsymbol{\varsigma}) : \ \mathbf{x} \in \mathcal{X}\} = n - 1 - \sum_{i=1}^{n-1} \left[\frac{(\varsigma_{i-1} + 2)^2}{4(\varsigma_i + 1)} + \frac{1}{2}\alpha^{-1}\varsigma_i^2 \right], \tag{2.7}$$

and we define $\varsigma_0 = 0$.

To solve the problem, the algorithm was programmed by Matlab using sequential quadratic programming method with active-set strategy and run on Intel(R) Core(TM) (1.20 GHz) Windows Vista(TM) personal notebook computer. We can easily obtain the global maximal solution of canonical dual problem $(\mathcal{P}^d)$ over $\mathcal{S}_a^+$ is $(0, \cdots, 0)$, and the global minimal solution to the primal problem $(\mathcal{P})$ is $(1, \cdots, 1)$. Table 1 presents the numerical results.

TABLE 2.1
Numerical results for distance geometry problem

n	CPU Time (Seconds)
50	0.64
100	0.77
500	20.89
1000	137.91
1500	522.45

The numerical results show that Rosenbrock function minimization problem can be solved precisely and efficiently by Canonical duality theory to obtain global optimal solutions.

3. Conclusions. We have presented a detailed application of the canonical duality theory for solving distance geometry problem. An analytical solution is obtained by the complementary-dual principle. Results show that by using the canonical dual transformation, the nonconvex primal problem can be converted to a concave maximization dual problem, which can be solved by well-developed convex minimization techniques. Application to sensor network localization problem shows that this NP-hard problem in global optimization is actually a special case of discretized finite deformation problem. The idea and the method presented in this article can be used and generalized to solve much more difficult problems in global optimization, network communication, and scientific computations. The development of techniques is essential to extrapolate the complexities of the real world. Comprehensive review of the canonical duality and its applications can be found in [6, 7, 9, 10, 13].

Acknowledgments. This paper was partially supported by a grant (AFOSR FA9550-10-1-0487) from the US Air Force Office of Scientific Research. Dr. Ning Ruan was supported by a funding from the Australian Government under the Collaborative Research Networks (CRN) program.

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