GLOBAL OPTIMAL SOLUTIONS TO NONCONVEX EUCLIDEAN DISTANCE GEOMETRY PROBLEMS

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EXTENDED 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.

Main results. We are interested in solving the following general nonlinear programming problem arising from Euclidean distance geometry:

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

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 $\mathbf{x}_j$, $(i,j) \in \mathcal{S} = \{1, 2, \cdots, n\}$; $\mathcal{X}_a \subset \mathbb{R}^{r\times n}$ is a feasible set; $\mathbf{T} = \{T_\alpha^i\} \in \mathcal{X}^* = \mathbb{R}^{n\times r}$ 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

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

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Introducing a linear (difference) operator $\mathbf{D} : \mathcal{X}_a \to \mathbb{R}^{r\times n\times n}$ such that

$$\mathbf{D}\mathbf{X} = \{\mathbf{X}(\mathbf{e}_i - \mathbf{e}_j)\} = \{\mathbf{x}_i - \mathbf{x}_j\}, \tag{0.1}$$

the canonical dual problem can be proposed as follows:

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

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. $G^\dagger(\boldsymbol{\varsigma})$ denotes the Moore-Penrose generalized inverse of $G(\boldsymbol{\varsigma})$, and

$$\mathbf{G}(\boldsymbol{\varsigma}) = \mathbf{A} + \mathbf{D}^T\boldsymbol{\varsigma}\mathbf{D};\ \ \mathbf{D}^T\boldsymbol{\varsigma} = (\mathbf{e}_i^T - \mathbf{e}_j^T)\boldsymbol{\varsigma}.$$

THEOREM 0.1 (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*

$$\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T} \tag{0.2}$$

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

$$\Pi(\bar{\mathbf{X}}) = \Pi^d(\bar{\varsigma}). \tag{0.3}$$

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

$$\nabla\Pi^d(\bar{\varsigma}) = \frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \mathbf{W}^{-1}\bar{\varsigma} - \boldsymbol{\mu} = 0, \tag{0.4}$$

where $\bar{\mathbf{X}} = \mathbf{G}^+(\bar{\varsigma})\mathbf{T}$. The criticality condition (0.4) is actually the canonical duality relation (constitutive equation), i.e., $\boldsymbol{\varsigma} = \mathbf{W}\circ(\frac{1}{2}(\mathbf{D}\bar{\mathbf{X}})^T(\mathbf{D}\bar{\mathbf{X}}) - \boldsymbol{\mu})$. 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

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

This proves the theorem. □

THEOREM 0.2. *Suppose that* $\bar{\varsigma}$ *is a critical point of the canonical dual function* $\Pi^d(\bar{\varsigma})$ *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* $\Pi(\mathbf{X})$ *on* $\mathbb{R}^{r\times n}$ *if and only if* $\bar{\varsigma}$ *is a global maximizer of* $\Pi^d(\varsigma)$ *on* $\mathcal{S}_a^+$*, i.e.,*

$$\Pi(\bar{\mathbf{X}}) = \min_{\mathbf{X}\in\mathbb{R}^{r\times n}} \Pi(\mathbf{X}) \Leftrightarrow \max_{\varsigma\in\mathcal{S}_a^+} \Pi^d(\varsigma) = \Pi^d(\bar{\varsigma}). \tag{0.5}$$

Proof. By Theorem 0.1 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

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

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

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

This proves the statement (0.5). □

REFERENCES

[1] A. Y. ALFAKIH, *Graph rigidity via Euclidean distance matrices*, Linear Algebra Appl., 310 (2000): pp. 149–165.

[2] A. Y. ALFAKIH, A. KHANDANI, AND H. WOLKOWICZ, *Solving Euclidean distance matris completion problems via Semidefinite programming*, Comput. Opt. and Appl., 12 (1999): pp. 13–30.

[3] A. BARVINOK , *Problems of distance geometry and convex properties of quadratic maps*, Disc. Comp. Geom., 13 (1995): pp. 189–202.

[4] P. BISWAS, T. C. LIANG, K. C. TOH, T. C. WANG, AND Y. Y. YE, *Semidefinite Programming Approaches for Sensor Network Localization with Noisy Distance Measurements*, IEEE T. on Autom. Sci. Eng., 3 (2006): pp. 360–371.

[5] D. Y. GAO, *Duality Principles in Nonconvex Systems: Theory, Methods and Applications*, Kluwer Academic Publishers, Dordrecht/Boston/London, 2000, xviii+454pp.

[6] D. Y. GAO AND N. RUAN, *Solutions and optimality criteria for nonconvex quadratic-exponential minimization problem*, Math. Method. of Oper. Res., 67 (2008), pp. 479–496.

[7] D. Y. GAO AND N. RUAN, *Solutions to quadratic minimization problems with box and integer constraints*, J. Global Optim., 47 (2010): pp. 463–484.

[8] D.Y. GAO, N. RUAN AND P.M. PARDALOS, *Canonical dual solutions to sum of fourth-order polynomials minimization problems with applications to sensor network localization*, in Sensors: Theory, Algorithms and Applications, V. L. Boginski, and C. W. Commander, P. M. Pardalos and Y. Y. Ye, eds., Springer, 61 (2012), pp. 37–54.

[9] D. Y. Gao, N. Ruan and H. D. Sherali, *Solutions and optimality criteria for nonconvex constrained global optimization problems*, J. Global Optim., 45 (2009): pp. 473–497.

[10] D. Y. Gao, N. Ruan and H. D. Sherali, *Canonical dual solutions for fixed cost quadratic program*, in Optimization and Optimal Control: Theory and Applications, A. Chinchuluun, P. M. Pardalos, R. Enkhbat and L. Tseveendorj, eds., Springer, 39 (2010): pp. 139–156.

[11] J. J. Moré and Z. J. Wu, *Global continuation for distance geometry problems*, SIAM Journal on Optim., 7 (1997): pp. 814–836.

[12] N. J. Wang, *Sum of squares method for sensor network localization*, Comput. Optim. Appl., 43 (2009): pp. 151–179.

[13] N. Ruan, D. C. Gao, and Y. Jiao, *Canonical dual least square method for solving general nonlinear systems of equations*, Comput. Optim. Appl., 47 (2010): pp. 335–347.

[14] J.Saxe, *Embeddability of weighted graphs in k-space is strongly NP-hard*, in Proc. 17th Allerton Conference in Communications, Control, and Computing, Monticello, IL, 1979: pp. 480–489.

[15] A.M. So and Y. Y. Ye, *A semidefinite programming approach to tensegrity theory and realizability of graphs*. Proceedings of the 17th Annual ACM-SIAM Symposium on Discrete Algorithms, 2006: pp. 766–775.

[16] P. Tseng, *Second-order cone programming relaxation of sensor network localization*, SIAM Journal on Optimization, 18 (2007): pp. 156–185.

[17] H. Waki, S. Kim, M. Kojima, and J. Muramatsu, *Sums of squares and semidefinite programming relaxations for polynomial optimization problems with structured sparsity*, SIAM J. Optimiz, 17 (2006): pp. 218–242.