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Conjugate-set game for a nonlinear programming problem [1]

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The conjugate point is a global concept in the calculus of variations. It plays a crucial role to guarantee optimality. Recently, a conjugate point theory was proposed for a minimization problem of a smooth function with n variables in [2] and [3], which matches Jacobi's classical conjugate point theory. In either theory, collaboration of variables is essential. Namely, even when a couple of variables can not improve a solution, collaboration of several variables may find a better solution. If such a set of variables exists, we call it a strict conjugate set. Then a simple question arises. How much does each variable of the strict conjugate set contribute to improve the solution? The aims of this paper are to emphasize a game-theoretic aspect of the conjugate point and to give an answer to the above question. To achieve the aims, we will define a cooperative game based on conjugate sets, which we call the conjugate-set game. Furthermore, we will compute the Shapley value for the conjugate-set game.

Keywords: Conjugate-set game, Conjugate set, Conjugate point, Collaboration, Cooperative game, Shapley value, Nonlinear programming problem

1 INTRODUCTION

The conjugate point was introduced by Jacobi to give a sufficient optimality condition for the simplest problem in the calculus of variations

$$(SP) \quad \text{Minimize} \quad \int_0^T f(t, x(t), \dot{x}(t))dt \quad \text{subject to} \quad x(0) = A,\ x(T) = B,$$

where A and B are given points in R^n, $T > 0$ fixed, and f is a smooth function. Conjugate points are defined as zero points of a non-trivial solution $y(t)$ of the Jacobi equation with the initial condition $y(0) = 0$. Jacobi proved that if a feasible solution $x(t)$ satisfies the Euler equation and the strengthened Legendre condition, and if there are no points conjugate to $t = 0$ on $[0, T]$, then $x(t)$ is a weak minimum for (SP), see e.g. [1].

Recently, a conjugate point theory was proposed for a minimization problem of a smooth function $f(x)$ with n variables

$$(P_0) \qquad \text{Minimize} \quad f(x), \quad x \in R^n$$

in [3]. The Jacobi equation for (P_0) is a difference equation that the descending principal minors of the Hesse matrix $f''(x)$ satisfy. According to Sylvester's criterion, an $n \times n$-symmetric matrix $A = (a_{ij})$ is positive-definite if and only if its descending principal minors $|A_k|$ $(k = 1, \ldots, n)$ are positive,

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where $A_k := (a_{ij})_{1\le i,\ j\le k}$, see e.g. [5]. Furthermore, $y_k := |A_k|$ satisfies the following recursion relation.

$$y_k = \sum_{i=0}^{k-1} \sum_{\rho\in S(i+1,k)} \varepsilon(\rho) a_{i+1\rho(i+1)} a_{i+2\rho(i+2)} \cdots a_{k\rho(k)} y_i, \quad k = 1,\dots,n, \tag{1.1}$$

where $y_0 := 1$, $\varepsilon(\rho)$ denotes the sign of ρ, and $S(k+1, n)$ denotes the set of all permutations ρ on $\{k+1,\dots,n\}$ satisfying that there is no $\ell > k$ such that ρ is closed on $\{\ell+1,\dots,n\}$. We call the recursion relation (1.1) the Jacobi equation for A. We say that k is (strictly) conjugate to 1 if the solution $\{y_i\}$ of the Jacobi equation with the initial condition $y_0 = 1$ changes the sign for the first time from positive to non-positive (negative) at k. Namely,

$$y_1 > 0,\ \dots,\ y_{k-1} > 0,\ \text{and } y_k \le 0 \quad (y_k < 0), \tag{1.2}$$

see [2]. Then, it is evident that A is positive definite if and only if there are no points conjugate to 1. Similarly, if there exists a number k such that k is strictly conjugate to 1, then A is not nonnegative definite.

By the way, since each variable x_k in (P_0) plays the same role in general, there are no reasons to start with $k = 1$ in order to define conjugate points. So it is natural to deal with $\{1,\dots,k\}$ or $\{x_1,\dots,x_k\}$ rather than the endpoints 1 and k. This idea leads us to a conjugate set and a cooperative game. We call the game the conjugate-set game.

This paper is organized as follows. In Section 2, we first define a conjugate set, and next present a fundamental theorem on conjugate sets. In Section 3, we introduce the conjugate-set game. We give several examples and compute their Shapley values.

2 Strict conjugate sets

In this section, we define (minimal strict) conjugate sets and give a fundamental theorem on conjugate sets.

DEFINITION **2.1** *Let $A = (a_{ij})$ be an $n \times n$ symmetric matrix, and $I = \{i_1,\dots,i_k\}$ a subset of $\{1,\dots,n\}$. If a submatrix $(a_{ij})_{i,j\in I}$ of A has a non-positive (negative) principal minor, then we call I a (strict) conjugate set. For the sake of convenience, we call the corresponding set of variables $\{x_k\}_{k\in I}$ a (strict) conjugate set. When any proper subset J of a (strict) conjugate set I is not a (strict) conjugate set, we call I (or $\{x_k\}_{k\in I}$) a minimal (strict) conjugate set.*

THEOREM **2.1** *Let $A = (a_{ij})$ be a $2m+1$-multi diagonal matrix, that is,*

$$a_{ij} = 0 \quad \textit{if} \quad |i-j| \ge m+1. \tag{2.1}$$

Then any number of any minimal (strict) conjugate set jumps at most m. In particular, when A is a tridiagonal matrix, any minimal (strict) conjugate set consists of sequential numbers.

Proof. Let I be an arbitrary minimal (strict) conjugate set. Assume that I is divided into non-empty sets I_1 and I_2 such that

$$j - i \geq m + 1 \quad \forall i \in I_1,\ \forall j \in I_2. \tag{2.2}$$

Denote by $S(I)$, $S(I_1)$, and $S(I_2)$ the set of permutations on I, I_1, and I_2, respectively. Denote by $A(I)$ the submatrix $(a_{ij})_{i,j\in I}$. Similarly, we define $A(I_1)$ and $A(I_2)$. Then, we get from (2.1) and (2.2) that $a_{i\sigma(i)} = 0$ for any $\sigma \in S(I)$ satisfying

$$\exists i \in I_1, \quad \sigma(i) \in I_2. \tag{2.3}$$

Hence, we may omit $\sigma \in S(I)$ satisfying (2.3) in the definition of $|A(I)|$. So,

$$|A(I)| = \sum_{\sigma\in S(I)} \varepsilon(\sigma) \prod_{i\in I} a_{i\sigma(i)} = \sum_{\sigma\in S(I),\ \sigma(I_1)=I_1} \varepsilon(\sigma) \prod_{i\in I} a_{i\sigma(i)}.$$

For such a $\sigma \in S_I$, we denote by σ_1 and σ_2 its restriction on I_1 and I_2, respectively. Then,

$$\begin{aligned} |A(I)| &= \sum_{\sigma\in S(I),\ \sigma(I_1)=I_1} \varepsilon(\sigma_1)\varepsilon(\sigma_2) \prod_{i\in I_1} a_{i\sigma_1(i)} \prod_{i\in I_2} a_{i\sigma_2(i)} \\ &= \left(\sum_{\sigma_1\in S(I_1)} \varepsilon(\sigma_1) \prod_{i\in I_1} a_{i\sigma_1(i)} \right) \left(\sum_{\sigma_2\in S(I_2)} \varepsilon(\sigma_2) \prod_{i\in I_2} a_{i\sigma_2(i)} \right) \\ &= |A(I_1)||A(I_2)|. \end{aligned}$$

Since I is a (strict) conjugate set, $|A(I)|$ is nonpositive (negative). Hence either $|A(I_1)|$ or $|A(I_2)|$ is nonpositive (negative), which contracts the minimality of I. This completes the proof.

EXAMPLE **2.1** *Let S_1 denote the sphere with center $(3/2, 0, 3/2)$ and radius $1/\sqrt{2}$, S_2 the sphere with center $(-3/2, 0, 3/2)$ and radius $1/\sqrt{2}$, and C the circle in $yz-$plane with center $(0, 0, R)$ and radius $R > 0$. Then our problem is to find $(X_1, X_2, X_3) \in S_1 \times S_2 \times C$ that minimizes the area of the triangle $X_1X_2X_3$. We may take as the objective function*

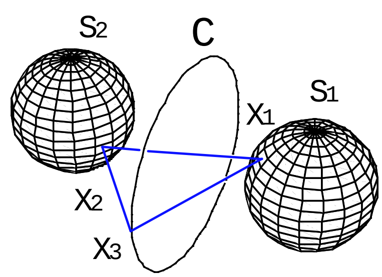

Figure 1: Minimal triangle 1

$$f(\theta_1, \phi_1, \theta_2, \phi_2, \theta_3) := \| (X_1 - X_3) \times (X_2 - X_3) \|^2 .$$

where

$$X_1 = \left(\frac{1}{\sqrt{2}} \sin\theta_1 \cos\phi_1 + \frac{3}{2}, \frac{1}{\sqrt{2}} \sin\theta_1 \sin\phi_1, \frac{1}{\sqrt{2}} \cos\theta_1 + \frac{3}{2} \right),$$

$$X_2 = \left(\frac{1}{\sqrt{2}} \sin\theta_2 \cos\phi_2 - \frac{3}{2}, \frac{1}{\sqrt{2}} \sin\theta_2 \sin\phi_2, \frac{1}{\sqrt{2}} \cos\theta_2 + \frac{3}{2} \right),$$

and

$$X_3 = (0, R\sin\theta_3, R\cos\theta_3 + R)$$

for some $0 \le \theta_1 \le \pi,\ 0 \le \phi_1 < 2\pi,\ 0 \le \theta_2 \le \pi,\ 0 \le \phi_2 < 2\pi,$ *and* $0 \le \theta_3 < 2\pi$. *We test whether* $(\bar{X}_1, \bar{X}_2, \bar{X}_3) := (1, 0, 1, -1, 0, 1, 0, 0, 0)$ *gives a minimal area*

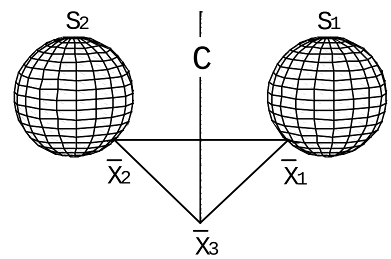

Figure 2: Minimal triangle 2

or not, that is, whether $\bar{\theta} := (\bar{\theta}_1, \bar{\phi}_1, \bar{\theta}_2, \bar{\phi}_2, \bar{\theta}_3) := (3\pi/4, \pi, 3\pi/4, 0, \pi)$ *is a local minimum of* f *or not. It is easily seen that* $\bar{\theta}$ *is a stationary point of* f *and that the Hesse matrix* $f''(\bar{\theta})$ *is given by*

$$\begin{pmatrix} 4 & 0 & -2 & 0 & 0 \\ 0 & 3 & 0 & 0 & -2R \\ -2 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 3 & 2R \\ 0 & -2R & 0 & 2R & 8R(R-1) \end{pmatrix}. \tag{2.4}$$

By exchanging the second row (column) with the third row (column), the Hesse matrix becomes

$$A := \begin{pmatrix} 4 & -2 & 0 & 0 & 0 \\ -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & -2R \\ 0 & 0 & 0 & 3 & 2R \\ 0 & 0 & -2R & 2R & 8R(R-1) \end{pmatrix}. \tag{2.5}$$

Since the descending principal minors of A *are given by*

$$|A_1| = 4,\ |A_2| = 12,\ |A_3| = 36,\ |A_4| = 108,\ |A_5| = 24R(2R-3),$$

$\bar{\theta}$ *is (not) minimal when* $R > 3/2$ $(R < 3/2)$. *In particular, when* $R < 1$, *since the last diagonal element* $8R(R-1)$ *is negative,* $\{\theta_3\}$ *is a minimal strict conjugate set, which implies that the area of the triangle gets bigger by changing* *only θ_3. On the other hand, when $1 < R < 3/2$, $\{\phi_1, \phi_2, \theta_3\}$ is a minimal strict conjugate set, which implies that a certain increment*

$$\Delta\theta := (\Delta\theta_1, \Delta\phi_1, \Delta\theta_2, \Delta\phi_2, \Delta\theta_3) = (0, \Delta\phi_1, 0, \Delta\phi_2, \Delta\theta_3)$$

decreases the objective function. Indeed, when $R = 5/4$ for example, by taking $\Delta\theta = (0, -\Delta\phi_1, 0, \Delta\phi_1, -\Delta\phi_1)$, we have

$$\begin{aligned} f(\bar{\theta} + \Delta\theta) &= (\cos\Delta\phi_1 - 3)^2(8\cos^2\Delta\phi_1 - 5\cos\Delta\phi_1 + 5) \\ &\simeq 32 - 6\Delta\phi_1^2 - \frac{\Delta\phi_1^4}{4} + O(\Delta\phi_1^5). \end{aligned}$$

Hence $f(\bar{\theta} + \Delta\theta) < f(\bar{\theta})$ for any sufficiently small $\Delta\phi_1$. Finally, we add a note from the view point of Theorem 2.1. If we number the variables $(\theta_1, \phi_1, \theta_2, \phi_2, \theta_3)$ as $(x_1, \ldots, x_5)$, then the indices corresponding to the minimal set $\{\phi_1, \phi_2, \theta_3\}$ are 2, 4 and 5, which jumps 1.

3 Conjugate-set game

In Example 2.1, we have just seen that if there exists a strict conjugate set, we can improve a solution by moving the variables of the strict conjugate set simultaneously. In this section, we give an answer to the question that how much does each variable of the strict conjugate set contribute to decrease the objective function. For this purpose, we define a cooperative game based on conjugate sets and compute its Shapley value.

DEFINITION **3.1** *For any subset S of $\{1, \ldots, n\}$, we define a characteristic function $v(S)$ by the maximum number $0 \leq k \leq n$ of disjoint strict conjugate sets contained in S. Let X denote the set of all variables $\{x_1, \ldots, x_n\}$. For any subset $X_S := \{x_i;\ i \in S\}$ of X, we defnie $v(X_S) := v(S)$. We call this cooperative game the conjugate-set game.*

The following lemma is obvious from the definition of $v(S)$.

LEMMA **3.1** (a) *$0 \leq v(S) \leq n$ for any S.* (b) *$v(\phi) = 0$.* (c) *If $S \cap T = \phi$, then $v(S) + v(T) \leq v(S \cup T)$.*

As is well-known, the Shapley value is defined by

$$\phi_i(v) = \sum_{i \in S} \frac{v(S) - v(S - \{i\})}{n \begin{pmatrix} n-1 \\ s-1 \end{pmatrix}}, \tag{3.1}$$

where s denotes the cardinal number of S. It is regarded as a measure to evaluate how much does player i contribute in the cooperative game with the characteristic function v.

EXAMPLE **3.1** *In Example 2.1, $\{\phi_1,\ \phi_2,\ \theta_3\}$ was the unique minimal strict conjugate set when $1 < R < 3/2$. So,*

$$v(Y) = \begin{cases} 1 & \textit{if} \quad \{\phi_1,\ \phi_2,\ \theta_3\} \subset Y, \\ 0 & \textit{if} \quad \{\phi_1,\ \phi_2,\ \theta_3\} \not\subset Y. \end{cases} \tag{3.2}$$

Then the Shapley value is given by

$$\phi_1(v) = \phi_3(v) = 0, \quad \phi_2(v) = \phi_4(v) = \phi_5(v) = \frac{1}{3}. \tag{3.3}$$

(3.3) is so expected. In order to present a non-trivial example, we consider the following extremal problem.

$$(P_1) \qquad \text{Minimize} \quad f(x) := \sum_{k=0}^{n} f_k(x_k, x_{k+1}), \quad x := (x_1, \ldots, x_n) \in R^n,$$

where x_0 and x_{n+1} are given. For example, the shortest polygonal path problem on a surface S is formulated as (P_1), see Example 3.2 below. Problem (P_1) has a nice property that the Hesse matrix is tridiagonal. So, the Jacobi equation (1.1) reduces to a recursion relation of three adjacent principal minors y_{k-2}, y_{k-1} and y_k. In [4], we analyzed conjugate points for constant tridiagonal Hesse matrices

$$A := \begin{pmatrix} a & b & & \\ b & a & \ddots & \\ & \ddots & \ddots & b \\ & & b & a \end{pmatrix}, \tag{3.4}$$

where a, $b \in R$. Without loss of generality, we may assume that $a > 0$ and $b = \pm 1$. Combining Theorem 2.1 and the main result of [4, Theorem 5.1], we get the following theorem.

THEOREM **3.1** *(a) When $a \geq 2$, there are no strict conjugate sets. (b) When $0 < a < 2$, let k denote the first number satisfying $(k+1)\varphi > \pi$, where φ $(0 < \varphi < \pi)$ is the argument of the solution of the characteristic equation*

$$y^2 - ay + 1 = 0. \tag{3.5}$$

If $k \leq n$, then $\{1, 2, \ldots, k\}, \{2, 3, \ldots, k+1\}, \ldots, \{n-k+1, n-k+2, \ldots, n\}$ are minimal strict conjugate sets.

Proof. (a) is a direct consequence of [4, Theorem 5.1]. (b): By [4, Theorem 5.1], when $0 < a < 2$, k is strictly conjugate to 1, which implies that $\{1, 2, \ldots, k\}$ is a strict conjugate set. On the other hand, by Theorem 2.1, any minimal strict conjugate set consists of a sequential numbers. Suppose that $\{1, 2, \ldots, k\}$ is not minimal. Then there exists a pair of numbers $(\ell, m) \neq (1, k)$ such that $\{\ell, \ell+1, \ldots, m\} (\subset \{1, 2, \ldots, k\})$ is a minimal strict conjugate set. So, we see from the form of A that $m - \ell + 1 (< k)$ is strictly conjugate to 1. This contradicts that k is strictly conjugate to 1.

EXAMPLE **3.2** *Let S be an ellipsoid defined by*

$$\frac{x^2}{a^2} + \frac{y^2}{a^2} + \frac{z^2}{c^2} = 1.$$

Let us find the shortest polygonal path joining two given points $A = (a, 0, 0)$ and $B = (a \cos T, a \sin T, 0)$, where $T > 0$ and each knot X_k is chosen from

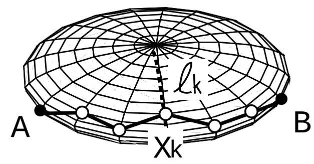

Figure 3: Shortest polygonal path problem

a longitude $\ell_k := \{(a\sin\theta\cos k\Delta t, a\sin\theta\sin k\Delta t, c\cos\theta) : 0 < \theta < \pi\}$ *and* $\Delta t := T/(n+1)$. *Since each knot is expressed as*

$$X_k = (a\sin\theta_k\cos k\Delta t,\ a\sin\theta_k\sin k\Delta t,\ c\cos\theta_k)$$

by some $0 < \theta_k < \pi$, *the length of* X_kX_{k+1}, *say* f_k, *is a function of* (θ_k, θ_{k+1}). *Hence the total length is given by* $f(\theta_1, \ldots, \theta_n) := \sum_{k=0}^{n} f_k(\theta_k, \theta_{k+1})$, *where* $\theta_0 = \theta_{n+1} := \pi/2$. *Next, let* $\bar{X}_k$ *denote the intersection of the equator and* ℓ_k. *Then* $\bar{\theta} := (\pi/2, \ldots, \pi/2)$ *corresponds to the equatorial polygonal path* $A\bar{X}_1 \cdots \bar{X}_nB$. *It is easily seen that* $\bar{\theta}$ *is a stationary point of* $f(\theta_1, \ldots, \theta_n)$. *Furthermore, since*

$$f_k''\left(\frac{\pi}{2}, \frac{\pi}{2}\right) = \frac{c^2}{2a\sin\frac{\Delta t}{2}}\begin{pmatrix} d & -1 \\ -1 & d \end{pmatrix}, \quad d := 1 - 2\frac{a^2}{c^2}\sin^2\frac{\Delta t}{2},$$

the Hesse matrix $f''\left(\frac{\pi}{2}, \ldots, \frac{\pi}{2}\right)$ *is equal to*

$$\frac{c^2}{2a\sin\frac{\Delta t}{2}}\begin{pmatrix} 2d & -1 & & \\ -1 & 2d & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2d \end{pmatrix}. \tag{3.6}$$

Since $0 < 2d < 2$ *for any sufficiently small* Δt, *this example reduces to case (b) of Theorem 3.1. So, denoting by* k *the first number satisfying* $(k+1)\varphi > \pi$, *where* $0 < \varphi < \pi$ *the argument of the solution of the characteristic equation* $y^2 - 2d + 1 = 0$, *we conclude that* $\{1, 2, \ldots, k\}, \{2, 3, \ldots, k+1\}, \ldots, \{n-k+1, n-k+2, \ldots, n\}$ *are minimal strict conjugate sets. As a special case, we consider the following two cases: (1)* $n = 5,\ k = 4$ *and (2)* $n = 9,\ k = 4$. *In*

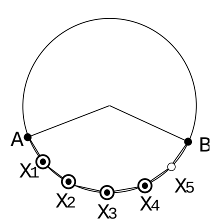

Figure 4: $n = 5,\ k = 4$

the case of $n = 5,\ k = 4$,

$$v(S) = \begin{cases} 1 & \text{if } S \text{ contains } \{1,2,3,4\} \text{ or } \{2,3,4,5\} \\ 0 & \text{otherwise.} \end{cases}$$

Hence

$$(\phi_1(v),\,\phi_2(v),\,\phi_3(v),\,\phi_4(v),\,\phi_5(v)) = \left(\frac{1}{20},\,\frac{6}{20},\,\frac{6}{20},\,\frac{6}{20},\,\frac{1}{20}\right).$$

In the case of $n = 9,\ k = 4$*, there are two disjoint minimal strict conjugate*

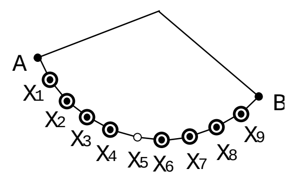

Figure 5: $n = 9,\ k = 4$

sets as Fig. 5. So,

$$v(S) = \begin{cases} 2 & \text{if } \ Y \supset \{1,2,3,4\} \cup \{6,7,8,9\} \\ 1 & \text{if } \ Y \text{ contains just one minimal strict conjugate set} \\ 0 & \text{otherwise.} \end{cases}$$

Therefore

$$(\phi_1(v),\ldots,\,\phi_9(v)) = \frac{1}{360}\,(23,\,86,\,104,\,122,\,50,\,122,\,104,\,86,\,23)\,,$$

which implies that X_5 *contributes less than* X_2, X_3, X_4, X_6, X_7 *and* X_8.

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