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RANK 1 CONVEX HULLS OF ISOTROPIC FUNCTIONS IN DIMENSION 2 BY 2

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Dedicated to Professor Jindřich Nečas on the occasion of his 70th birthday

Abstract. Let f be a rotationally invariant (with respect to the proper orthogonal group) function defined on the set $\mathrm{M}^{2\times 2}$ of all 2 by 2 matrices. Based on conditions for the rank 1 convexity of f in terms of signed invariants of $\mathbf{A}$ (to be defined below), an iterative procedure is given for calculating the rank 1 convex hull of a rotationally invariant function. A special case in which the procedure terminates after the second step is determined and examples of the actual calculations are given.

Keywords: rank 1 convexity, relaxation, stored energies

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1. Introduction

Let $\mathrm{M}^{2\times 2}$ denote the linear space of all 2 by 2 matrices. A function $f\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ is said to be rotationally invariant (briefly, invariant) if $f(\mathbf{A}) = f(\mathbf{RAQ})$ for all $\mathbf{A} \in \mathrm{M}^{2\times 2}$ and all $\mathbf{Q}, \mathbf{R}$ proper orthogonal. A rotationally invariant function has a representation

$$f(\mathbf{A}) = \tilde{f}(w) \tag{1}$$

where $\tilde{f}$ is a symmetric function on $\mathbb{R}^2$ and $w = (w_1, w_2)$ are the signed singular values of $\mathbf{A}$, defined ([7], [10]) as the unique pair such that $w_1 \geqslant |w_2|$ are ordered eigenvalues, with appropriate multiplicities, of $\sqrt{\mathbf{A}\mathbf{A}^T}$, and $\operatorname{sgn} w_2 = \operatorname{sgn}\det\mathbf{A}$.

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We write $\widehat{w}(\mathbf{A}) = (\widehat{w}_1(\mathbf{A}), \widehat{w}_2(\mathbf{A}))$ for the signed singular values of $\mathbf{A}$. A function $f\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ is said to be rank 1 convex if it is convex on each closed line segment $[\mathbf{A}, \mathbf{B}]$, $\mathbf{A}, \mathbf{B} \in \mathrm{M}^{2\times 2}$, such that $\operatorname{rank}(\mathbf{A} - \mathbf{B}) \leqslant 1$. The rank 1 convexity and the closely related notions of quasiconvexity and polyconvexity play important roles as necessary or sufficient conditions on f for the existence of solutions (minimizers of energy) in the calculus of variations [6], [3], nonlinear elasticity [1], and theory of phase transitions, see e.g. [4], [8], [9]. When the stored energy f fails to be quasiconvex, the effective energy of the system is represented by the quasiconvex hull (= the relaxation) $Qf\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ of f, defined as the largest quasiconvex function not exceeding f. Closely related to Qf are also the rank 1 convex and polyconvex hulls Rf and Pf, defined as the largest rank 1 convex and polyconvex functions not exceeding f. One has $Pf \leqslant Qf \leqslant Rf$ and it may happen (as the experience shows) that $Pf = Rf$, thereby determining also Qf, which is otherwise difficult.

This paper deals with rank 1 convex hulls of rotationally invariant functions. By the results of [10], the rank 1 convexity of an invariant f takes the form of a restricted ordinary convexity on certain cones $K^{\pm}$ when f is represented in terms of signed invariants (see Section 2 for definitions). Using this, a limiting procedure is given for finding the rank 1 convex hull of a rotationally invariant function, similar to the construction of the rank 1 convex hull of a general function (with no invariance property) by Kohn and Strang [5]. The difference is that the procedure is defined in the 2-dimensional space of signed invariants, while in the case of [5] in the 4-dimensional space of matrices. Each step requires to find a minimum of convex combinations of the preceding step with the given barycenter, restricted to $K^{\pm}$, and then to apply certain monotonization of the result. Finally, the case when the procedure terminates after the second step is determined, and two examples, one of which resembles an isotropic double well potential, are given.

2. Invariant rank 1 convex functions

Let $\widehat{X}_{\pm}\colon \mathrm{M}^{2\times 2} \to \mathbb{R}^2$ be mappings defined by

$$\widehat{X}_{\pm}(\mathbf{A}) = \bigl(\sqrt{|\mathbf{A}|^2 \pm 2\det \mathbf{A}}, \det \mathbf{A}\bigr), \quad \mathbf{A} \in \mathrm{M}^{2\times 2}.$$

We say that $\widehat{X}_+$ associates, with a given $\mathbf{A} \in \mathrm{M}^{2\times 2}$, the pair $x = (x_1, x_2) := \widehat{X}_+(\mathbf{A})$ of +signed invariants of $\mathbf{A}$, and $\widehat{X}_-$ the pair $y = (y_1, y_2) := \widehat{X}_-(\mathbf{A})$ of −signed invariants of $\mathbf{A}$. We have

$$x_1 = w_1 + w_2, \quad x_2 = w_1 w_2, \tag{2}$$

$$y_1 = w_1 - w_2, \quad y_2 = w_1 w_2, \tag{3}$$

where (w_1, w_2) are the signed singular values of $\mathbf{A}$ as defined in Introduction. Note that as a consequence of (2), (3) we have

$$y_1 = \sqrt{x_1^2 - 4x_2}, \quad y_2 = x_2. \tag{4}$$

The mappings $\widehat{X}_\pm$ map $\mathrm{M}^{2\times 2}$ onto $Q_\pm$, respectively, where

$$Q_+ := \{(x_1, x_2) \in \mathbb{R}^2 \colon\ x_1 \geqslant 0,\ x_2 \leqslant \tfrac{1}{4}x_1^2\},$$

$$Q_- := \{(y_1, y_2) \in \mathbb{R}^2 \colon\ y_1 \geqslant 0, y_2 \geqslant -\tfrac{1}{4}y_1^2\}.$$

If $\mathbf{A}, \mathbf{B} \in \mathrm{M}^{2\times 2}$, then

$$\widehat{X}_+(\mathbf{A}) = \widehat{X}_+(\mathbf{B}) \quad \Leftrightarrow \quad \mathbf{A} = \mathbf{QBR} \quad \text{for some} \quad \mathbf{Q}, \mathbf{R} \in \mathrm{SO}(2),$$

and a similar equivalence holds with $\widehat{X}_+$ replaced by $\widehat{X}_-$. See [10] for details. It follows that any rotationally invariant function $f\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ has a representation $\tilde{f}^+\colon Q_+ \to \mathbb{R}$ in terms of the $+$signed invariants such that

$$f(\mathbf{A}) = \tilde{f}^+(\widehat{X}_+(\mathbf{A})), \quad \mathbf{A} \in \mathrm{M}^{2\times 2},$$

and a representation $\tilde{f}^-\colon Q_- \to \mathbb{R}$ in terms of the $-$signed invariants such that

$$f(\mathbf{A}) = \tilde{f}^-(\widehat{X}_-(\mathbf{A})), \quad \mathbf{A} \in \mathrm{M}^{2\times 2}.$$

The importance of $\tilde{f}^\pm$ derives from the fact that the rank 1 convexity of f takes the form of a restricted ordinary convexity of $\tilde{f}^\pm$ on certain cones $K^\pm$ in $Q_\pm$. These cones are defined as follows. For each $x \in Q_+$,

$$K^+(x) := \{x + (t, st)\colon\ w_2 \leqslant s \leqslant w_1,\ t \in \mathbb{R},\ x + (t, st) \in Q_+\},$$

where (w_1, w_2) are uniquely determined by (2); for each $y \in Q_-$,

$$K^-(y) := \{y + (t, st)\colon\ -w_1 \leqslant s \leqslant w_2,\ t \in \mathbb{R},\ x + (t, st) \in Q_-\}$$

where (w_1, w_2) are uniquely determined by (3). The reader is referred to [10; Figures 1(b), 2(b)] for the pictures of $K^+(x)$ and $K^-(y)$. Furthermore, for each $p \equiv x \in Q_+$ or $p \equiv y \in Q_-$ we denote

$$A_\pm(p) = \{(\alpha, z) \in \mathbb{R}^2\colon\ 0 \leqslant \alpha \leqslant 1,\ p + (1-\alpha)z,\ p - \alpha z \in K^\pm(p)\}.$$

Each $(\alpha, z) \in A_+(x)$ determines a decomposition of $x \in Q_+$ in the form

$$x = \alpha\tilde{x} + (1-\alpha)\bar{x},$$

where $\tilde{x} = x + (1-\alpha)z$, $\bar{x} = x - \alpha z$, $\tilde{x}$, $\bar{x} \in K^+(x)$. A similar interpretation applies to $A_-(y)$.

2.1 Proposition. *An invariant function f is rank 1 convex if and only if the following two conditions hold simultaneously:*

(a) *$\tilde{f}^+$ is nondecreasing in the first variable and for each $x \in Q_+$ we have*

$$\tilde{f}^+(x) \leqslant \alpha\tilde{f}^+(x + (1-\alpha)z) + (1-\alpha)\tilde{f}^+(x - \alpha z) \tag{5}$$

whenever $(\alpha, z) \in A_+(x)$;

(b) *$\tilde{f}^-$ is nondecreasing in the first variable and for each $y \in Q_-$ we have*

$$\tilde{f}^-(y) \leqslant \alpha\tilde{f}^-(y + (1-\alpha)z) + (1-\alpha)\tilde{f}^-(y - \alpha z) \tag{6}$$

whenever $(\alpha, z) \in A_-(y)$.

Proof. If f is continuously differentiable, this is just a reformulation of [10; Proposition 6.2]. The general case is treated similarly, and the details are omitted. □

3. Rank 1 convex hulls of invariant functions

Note that if f is rotationally invariant then the rank 1 convex hull Rf is rotationally invariant, see [2], [11]. In this section we describe an iterative procedure $V^k f, k \to \infty$, for the construction of Rf. Another procedure will be described in [11].

The operations $M^\pm, S^\pm$ to be now introduced are motivated by the form of Conditions (a), (b) of Proposition 2.1. For each $f\colon Q_+ \to \mathbb{R}$ we denote by $M^+f\colon Q_+ \to \mathbb{R}, S^+f\colon Q_+ \to \mathbb{R}$ the functions defined by

$$\begin{aligned} M^+f(x) &= \inf\{f(t, x_2)\colon\ t \geqslant x_1\},\\ S^+f(x) &= \inf\{\alpha f(x + (1-\alpha)z) + (1-\alpha)f(x - \alpha z)\colon\ (\alpha, z) \in A_+(x)\}, \end{aligned}$$

$x \in Q_+$. Clearly, $M^+f \leqslant f, S^+f \leqslant f$; M^+f is the largest function nondecreasing in the first variable not exceeding f. Similarly, for each $f\colon Q_- \to \mathbb{R}$ we denote by $M^-f\colon Q_- \to \mathbb{R}, S^-f\colon Q_- \to \mathbb{R}$ the functions defined by

$$\begin{aligned} M^-f(y) &= \inf\{f(t, y_2)\colon\ t \geqslant y_1\},\\ S^-f(y) &= \inf\{\alpha f(y + (1-\alpha)z) + (1-\alpha)f(y - \alpha z)\colon\ (\alpha, z) \in A_-(y)\}, \end{aligned}$$

$y \in Q_-$. Let f be an invariant function and define a function $Vf\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ by

$$Vf(\mathbf{A}) = \min\{M^+S^+\tilde{f}^+(x), M^-S^-\tilde{f}^-(y)\}, \quad \mathbf{A} \in \mathrm{M}^{2\times 2},$$

where x, y are given by (2) and $\tilde{f}^\pm$ are the representations of f in terms of the signed invariants. We have

$$Rf \leqslant Vf \leqslant f$$

where we use Proposition 2.1.

3.1 Theorem. *Let f be an invariant function, bounded from below by a rank 1 convex function and define a sequence f_k, $k = 0, \ldots$, by $f_0 = f$, $f_{k+1} = Vf_k$. Then*

$$Rf = \lim_{k\to\infty} f_k. \tag{7}$$

Proof. The sequence f_k is nonincreasing and so the limit g in (7) exists; since f is bounded from below by a rank 1 convex function, g is finite. We shall verify that g satisfies the conditions of Proposition 2.1. Let $\tilde{f}_k^\pm, \tilde{g}^\pm$ be the representations of f_k, g. For any $x \in Q_+, y \in Q_-$ related by (4) we have

$$\tilde{f}_{k+1}^+(x) = \tilde{f}_{k+1}^-(y) = \min\{M^+S^+\tilde{f}_k^+(x), M^-S^-\tilde{f}_k^-(y)\}. \tag{8}$$

By the construction, the functions $M^+S^+\tilde{f}_k^+(x), M^-S^-\tilde{f}_k^-(y)$ are nondecreasing with respect to their first variables x_1, y_1, respectively. By (4), $M^-S^-\tilde{f}_k^-(y)$ can be expressed as a function of x and the form of (4) shows that then $x \mapsto M^-S^-\tilde{f}_k^-(y)$ is a nondecreasing function in x_1. Thus by (8), $\tilde{f}_{k+1}^+(x)$ is the minimum of two functions nondecreasing in x_1 and hence so is also $\tilde{f}_{k+1}^+$. The same applies to $\tilde{f}_{k+1}^-$ and y_1. This in turn implies that $\tilde{g}^\pm$, being the limits of $\tilde{f}_k^\pm$, are nondecreasing in their first variables. Thus g satisfies the monotonicity requirements in Proposition 2.1. Thus it remains to verify (5) and (6). For each k and $(\alpha, z) \in A_\pm(x)$ we have

$$\tilde{f}_{k+1}^\pm(x) \leqslant \alpha\tilde{f}_k^\pm(x + (1-\alpha)z) + (1-\alpha)\tilde{f}_k^\pm(x - \alpha z).$$

Taking the limit, we obtain

$$\tilde{g}^\pm(x) \leqslant \alpha\tilde{g}^\pm(x + (1-\alpha)z) + (1-\alpha)\tilde{g}^\pm(x - \alpha z).$$

□

In this section we describe an elementary case when the procedure described in Theorem 3.1 terminates after a few steps, and apply the results to examples. The main feature of the special case is that the representations $\tilde{f}^{\pm}$ are of the separated form in the variables x_1, x_2 or y_1, y_2.

4.1 Proposition. *Let* $f_\pm\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ *be defined by*

$$f_\pm(\mathbf{A}) = \psi(s_\pm) + \gamma \det \mathbf{A}$$

where

$$s_\pm = \sqrt{|\mathbf{A}|^2 \pm 2\det \mathbf{A}},$$

$\psi\colon [0,\infty) \to \mathbb{R}$ *is bounded from below, and* $\gamma \in \mathbb{R}$. *Then*

$$Rf_\pm(\mathbf{A}) = Pf_\pm(\mathbf{A}) = \psi_0(s_\pm) + \gamma \det \mathbf{A}$$

where $\psi_0\colon [0,\infty) \to \mathbb{R}$ *is the largest convex nondecreasing function not exceeding* ψ.

Proof. Let us consider only f_+, which we denote by f; the treatment of f_- is similar. Consider the sequence f_k defined in Theorem 3.1 and denote by $\tilde{f}_k^{\pm}$ the corresponding representations in terms of the signed invariants. Let us show that

$$\begin{aligned}
\tilde{f}_0^+(x) &= \psi(x_1) + \gamma x_2,\\
\tilde{f}_1^+(x) &= \psi_0(x_1) + \gamma x_2,\\
\tilde{f}_k^+(x) &= \tilde{f}_1^+(x), \quad k \geqslant 1.
\end{aligned}$$

The expression for $\tilde{f}_0^+$ is just the representation of f. To obtain the expression for $\tilde{f}_1^+$, let $\psi_1\colon (0,\infty) \to \mathbb{R}$ be the convexification of ψ. Let $x \in Q_+$ be such that $x_2 > 0$. Then

$$\begin{aligned}
S^+\tilde{f}_0^+(x) &= \inf\{\alpha\tilde{f}_0^+(x + (1-\alpha)z) + (1-\alpha)\tilde{f}_0^+(x - \alpha z)\colon (\alpha, z) \in A_+(x)\}\\
&= \inf\{\alpha\psi(x_1 + (1-\alpha)z_1) + (1-\alpha)\psi(x_1 - \alpha z_1) + \gamma x_2\colon (\alpha, z) \in A_+(x)\}\\
&= \psi_1(x_1) + \gamma x_2.
\end{aligned}$$

Next we have to apply the monotonization operator M^+ to $\psi_1(x_1) + \gamma x_2$, which leads to $\psi_0(x_1) + \gamma x_2$ and hence the expression for $\tilde{f}_1^+$ is proved. The proof is now completed by noting that $\tilde{f}_1^+$ represents a polyconvex function. This follows from the fact that $\mathbf{A} \mapsto \widehat{w}_1(\mathbf{A}) \pm \widehat{w}_2(\mathbf{A})$, $\mathbf{A} \in \mathrm{M}^{2\times 2}$, is convex, see [9], [7], [10]. □

4.2 Example. Let $f\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ be given by

$$f(\mathbf{A}) = (\widehat{w}_1(\mathbf{A}) - a)^2 + (\widehat{w}_2(\mathbf{A}) - a)^2, \quad \mathbf{A} \in \mathrm{M}^{2\times 2},$$

where $a > 0$. Then

$$Rf(\mathbf{A}) = Pf(\mathbf{A}) = \begin{cases} a^2 - 2\det\mathbf{A} & \text{if} \quad \sqrt{|\mathbf{A}|^2 + 2\det\mathbf{A}} \leqslant a, \\ f(\mathbf{A}) & \text{if} \quad \sqrt{|\mathbf{A}|^2 + 2\det\mathbf{A}} \geqslant a. \end{cases}$$

This example shows that even though f is represented by a convex function of the signed singular values of the well form, f is not rank 1 convex. The reason is that in the region $w_1 + w_2 \leqslant a$, the function f violates the Baker-Ericksen inequalities.

Proof. One finds that

$$f(\mathbf{A}) = \psi(\widehat{w}_1(\mathbf{A}) + \widehat{w}_2(\mathbf{A})) - 2\det\mathbf{A},$$

where

$$\psi(t) = (t-a)^2 + a^2, \quad t \geqslant 0.$$

The function Rf is calculated in 4.1, and we find that the largest convex nondecreasing function ψ_0 not exceeding ψ is

$$\psi_0(t) = \begin{cases} a^2 & \text{if} \quad 0 \leqslant t \leqslant a, \\ (t-a)^2 + a^2 & \text{if} \quad t \geqslant a. \end{cases}$$

This completes the proof. $\square$

4.3 Example. Let $f\colon \mathrm{M}^{2\times 2} \to \mathbb{R}$ be given by

$$f(\mathbf{A}) = \min\{f_1(\mathbf{A}), f_2(\mathbf{A})\}, \quad \mathbf{A} \in \mathrm{M}^{2\times 2},$$

where

$$f_1(\mathbf{A}) = (\widehat{w}_1(\mathbf{A}) - a)^2 + (\widehat{w}_2(\mathbf{A}) - a)^2, \quad f_2(\mathbf{A}) = (\widehat{w}_1(\mathbf{A}) - b)^2 + (\widehat{w}_2(\mathbf{A}) - b)^2,$$

where $0 < a < b$, i.e.,

$$f(\mathbf{A}) = \begin{cases} f_1(\mathbf{A}) & \text{if} \quad s(\mathbf{A}) \leqslant a + b, \\ f_2(\mathbf{A}) & \text{if} \quad s(\mathbf{A}) > a + b, \end{cases}$$

where

$$s(\mathbf{A}) = \widehat{w}_1(\mathbf{A}) + \widehat{w}_2(\mathbf{A}).$$

Then

$$Rf(\mathbf{A}) = Pf(\mathbf{A}) = \begin{cases} a^2 - 2\det\mathbf{A} & \text{if} \quad s(\mathbf{A}) \leqslant a, \\ f_1(\mathbf{A}) & \text{if} \quad a \leqslant s(\mathbf{A}) \leqslant \frac{1}{2}(3a+b), \\ (a+b)s(\mathbf{A}) + c - 2\det\mathbf{A} & \text{if} \quad \frac{1}{2}(3a+b) \leqslant s(\mathbf{A}) \leqslant \frac{1}{2}(a+3b), \\ f_2(\mathbf{A}) & \text{if} \quad s(\mathbf{A}) \geqslant \frac{1}{2}(a+3b), \end{cases}$$

where

$$c = a^2 - \tfrac{1}{4}(a+b)(5a+b).$$

This is a relaxation of a "double well potential."

P r o o f. We have

$$f(\mathbf{A}) = \psi(s(\mathbf{A})) - 2\det\mathbf{A}, \quad \mathbf{A} \in \mathrm{M}^{2\times 2},$$

where

$$\psi(t) = \begin{cases} (t-a)^2 + a^2 & \text{if} \quad 0 < t \leqslant a+b, \\ (t-b)^2 + b^2 & \text{if} \quad t \geqslant a+b, \end{cases}$$

and

$$Rf(\mathbf{A}) = Pf(\mathbf{A}) = \psi_0(s(\mathbf{A})) - 2\det\mathbf{A}, \quad \mathbf{A} \in \mathrm{M}^{2\times 2}$$

where ψ_0 is the largest nondecreasing function not exceeding ψ. We have

$$\psi_0(t) = \begin{cases} a^2 & \text{if} \quad 0 < t \leqslant a, \\ (t-a)^2 + a^2 & \text{if} \quad a \leqslant t \leqslant \frac{1}{2}(3a+b), \\ (a+b)t + c & \text{if} \quad \frac{1}{2}(3a+b) \leqslant t \leqslant \frac{1}{2}(a+3b), \\ (t-b)^2 + b^2 & \text{if} \quad t \geqslant \frac{1}{2}(a+3b). \end{cases}$$

The proof is complete. □

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