Necessary and sufficient conditions for strong ellipticity of isotropic functions in any dimension

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Abstract

We consider hyperelastic stored energy functions in $\mathbb{R}^{n \times n}$ that are isotropic. We give necessary and sufficient conditions for the ellipticity of such functions. The present article is essentially a review of recent results on the subject

1 Introduction

Let $\mathbb{R}^{n \times n}_+$ be the set of $n \times n$ matrices whose determinant is positive. Consider a C^2 function $f : \mathbb{R}^{n \times n}_+ \to \mathbb{R}$ such that

$$f(F) = g(\lambda_1(F), ..., \lambda_n(F)) \tag{1}$$

for a certain symmetric $g : \mathbb{R}^n_+ \to \mathbb{R}$ and where $\lambda_i(F)$ stands for the singular values of F (i.e. the eigenvalues of $(F^T F)^{1/2}$).

The aim of the present article is to give necessary and sufficient conditions on g so that f satisfies the *ellipticity* (or *Legendre-Hadamard*) condition

$$\sum_{i,j,k,l=1}^{n} \frac{\partial^2 f(F)}{\partial F_{ik} \partial F_{jl}} \alpha_i \alpha_j \beta_k \beta_l \geq 0 \tag{2}$$

for every $\alpha, \beta \in \mathbb{R}^n$ and every $F \in \mathbb{R}^{n \times n}_+$. As a consequence we will also have results for *strong ellipticity*, which means that (2) holds with a strict inequality whenever $|\alpha|, |\beta| \neq 0$.

We now present the motivations for such a study. In nonlinear elasticity the function f is called the stored energy function, F is the deformation gradient and $\lambda_i(F)$ are the principal stretches. Many elastic materials are *isotropic* which, combined with the requirement that f is objective, means that

$$f(FR) = f(QF) = f(F), \ \forall F \in \mathbb{R}^{n \times n}_+, \ \forall Q, R \in SO(n)$$

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where $SO(n)$ stands for the set of orthogonal matrices with positive determinant. It turns out that these assumptions are equivalent to the existence of a function g such that (1) holds.

One also usually requires that the stored energy function f is either *convex* (which seems to be, in general, not physically realistic), or *polyconvex* or *rank one convex*. The last one is equivalent, when f is C^2, to the ellipticity condition mentioned above. Hill [13], Thompson and Freede [20] and Ball [5] gave necessary and sufficient conditions on g for the convexity of f while Ball in [5] dealt with the polyconvexity of f (see also for both cases Le Dret [15] and Dacorogna-Marcellini [10]). The same was achieved by Knowles and Sternberg [14] for rank one convexity only in the plane (i.e. when $n = 2$). This last result was then proved in a different manner by Aubert [1], Aubert and Tahraoui [3], Ball [6], Davies [11] and Dacorogna and Marcellini [10]. When $n = 3$ Aubert and Tahraoui in [2] gave also some necessary conditions and, although in a slightly different context, necessary and sufficient conditions were derived by Simpson and Spector [19] (see also Zee and Sternberg [21]). Finally Silhavy [18] established the result in any dimension but in terms of the copositivity of some matrices.

We here combine the result of Silhavy with one of Hadeler [12] on copositive matrices in dimension 3 and we will also give some simpler sufficient conditions in general dimension. The necessary and sufficient conditions for rank one convexity when $n = 3$ are now discussed. The first set of conditions is (letting $g_i = \partial g / \partial x_i$, $g_{ij} = \partial^2 g / \partial x_i \partial x_j$)

$$g_{ii} \geq 0,\ i = 1, 2, 3 \tag{3}$$

$$\frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i - \lambda_j} \geq 0,\ \lambda_i \neq \lambda_j,\ 1 \leq i < j \leq 3 \tag{4}$$

and express for the first ones the convexity of g with respect to each variable separately, while the second ones are equivalent to the *Baker-Ericksen inequalities* [4] and are also valid in any dimension. Actually these conditions are the easiest to derive and were known before the different works that we mentioned above. The last set of conditions read as follows for $\lambda_i \neq \lambda_j$ (if $\lambda_i = \lambda_j$ these inequalities are still valid when properly interpreted, cf. below)

$$\sqrt{g_{ii}g_{jj}} + m_{ij}^{\varepsilon} \geq 0,\ 1 \leq i < j \leq 3 \tag{5}$$

(these are identical to those from the case $n = 2$) and either

$$m_{12}^{\varepsilon}\sqrt{g_{33}} + m_{13}^{\varepsilon}\sqrt{g_{22}} + m_{23}^{\varepsilon}\sqrt{g_{11}} + \sqrt{g_{11}g_{22}g_{33}} \geq 0 \tag{6}$$

or

$$\det M^{\varepsilon} \geq 0 \tag{7}$$

where $M^{\varepsilon} = \left(m_{ij}^{\varepsilon}\right)$ with

$$m_{ij}^{\varepsilon} = \begin{cases} g_{ii} & \text{if } i = j \\ \varepsilon_i \varepsilon_j g_{ij} + \frac{g_i - \varepsilon_i \varepsilon_j g_j}{\lambda_i - \varepsilon_i \varepsilon_j \lambda_j} & \text{if } i \neq j \end{cases}$$

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and for any choice of $\varepsilon_i \in \{\pm 1\}$.

Note that there are 3 inequalities in (3), 3 in (4) and 12 in (5). However, since g is symmetric, it is enough to establish only 6 of them, for example those with $i = 1$ and $j = 2$. Due to all possible signs we have 4 equations in (6) or in (7).

2   Main result

We will let

$$\begin{aligned}
\mathbb{R}_+^n &= \{x \in \mathbb{R}^n : x_i > 0, \ i = 1, ..., n\} \\
\mathbb{R}_+^{n \times n} &= \{A \in \mathbb{R}^{n \times n} : \det A > 0\}.
\end{aligned}$$

A function $g : \mathbb{R}_+^n \to \mathbb{R}$ will be said to be symmetric if for every $x \in \mathbb{R}_+^n$ and for every permutation P of n elements the following holds

$$g(Px) = g(x).$$

We also need he following definition (cf. Motzkin [16], see also Hadeler [12] for an extended bibliography).

Definition 1 *A matrix $A \in \mathbb{R}^{n \times n}$ is said to be copositive if*

$$\langle Ax; x \rangle \geq 0, \ \forall x \in \mathbb{R}^n \ with \ x_i \geq 0, \ i = 1, ..., n.$$

It will be said to be strictly copositive if the inequality is strict whenever $x_i \geq 0$ and $x \neq 0$.

We start with a lemma which holds in any dimension and that was established by Silhavy [18], Proposition 6.4 (cf. also [19]). We give here his proof.

Lemma 2 *Let*
$$f(F) = g(\lambda_1(F), ..., \lambda_n(F))$$
where $g \in C^2(\mathbb{R}_+^n)$ and g is symmetric. Then $f : \mathbb{R}_+^{n \times n} \to \mathbb{R}$ is rank one convex if and only if the following two sets of conditions hold for every $\lambda \in \mathbb{R}_+^n$

$$\frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i - \lambda_j} \geq 0, \ \lambda_i \neq \lambda_j, \ 1 \leq i < j \leq n \tag{8}$$

$$M^\varepsilon = (m_{ij}^\varepsilon)_{1 \leq i,j \leq n} \ \ is \ copositive \tag{9}$$

where M^ε is symmetric and

$$m_{ij}^\varepsilon = \begin{cases} g_{ii} & if \ i = j \ or \ if \ i < j \ and \ \lambda_i = \lambda_j \\ \varepsilon_i \varepsilon_j g_{ij} + \frac{g_i - \varepsilon_i \varepsilon_j g_j}{\lambda_i - \varepsilon_i \varepsilon_j \lambda_j} & if \ i < j \ and \ \lambda_i \neq \lambda_j \ or \ \varepsilon_i \varepsilon_j \neq 1 \end{cases}$$

and for any choice of $\varepsilon_i \in \{\pm 1\}$.

Remark 3 *The proof of the lemma also shows that strong ellipticity is equivalent to the conditions (8) with strict inequalities and to the strict copositivity of M^ε.*

Proof. As well known the function f is rank one convex if and only if the Legendre-Hadamard condition holds, namely

$$L = \sum_{i,j,k,l=1}^{n} \frac{\partial^2 f(F)}{\partial F_{ik} \partial F_{jl}} \alpha_i \alpha_j \beta_k \beta_l \geq 0$$

for every $\alpha, \beta \in \mathbb{R}^n$ and every $F \in \mathbb{R}_+^{n \times n}$. According to Ball (Theorem 6.4 in [6], see also [7], [8]) if $\lambda_i(F) > 0$ and all different then

$$L = \sum_{i,j=1}^{n} g_{ij} \alpha_i \alpha_j \beta_i \beta_j + \sum_{i \neq j} G_{ij} \alpha_i^2 \beta_j^2 + \sum_{i \neq j} H_{ij} \alpha_i \alpha_j \beta_i \beta_j$$

where

$$G_{ij} = \frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i^2 - \lambda_j^2}, \; H_{ij} = \frac{\lambda_j g_i - \lambda_i g_j}{\lambda_i^2 - \lambda_j^2}.$$

Note that when $\lambda_i = \lambda_j$ the symmetry of g (which implies that at $\lambda_i = \lambda_j$ $g_i = g_j$ and $g_{ii} = g_{jj}$) allows us to interpret G_{ij} and H_{ij} as

$$G_{ij} = \frac{1}{2} \left[g_{ii} - g_{ij} + \frac{g_i}{\lambda_i} \right], \; H_{ij} = \frac{1}{2} \left[g_{ii} - g_{ij} - \frac{g_i}{\lambda_i} \right].$$

We rewrite L as

$$\begin{aligned} L &= \sum_{i=1}^{n} g_{ii} (\alpha_i \beta_i)^2 + 2 \sum_{i<j} [\varepsilon_i \varepsilon_j g_{ij} + G_{ij} + \varepsilon_i \varepsilon_j H_{ij}] \varepsilon_i \varepsilon_j \alpha_i \alpha_j \beta_i \beta_j \\ &\quad + \sum_{i<j} G_{ij} (\alpha_i \beta_j - \varepsilon_i \varepsilon_j \alpha_j \beta_i)^2 . \end{aligned}$$

Note that since

$$m_{ij}^\varepsilon = \begin{cases} g_{ii} & \text{if } i = j \\ \varepsilon_i \varepsilon_j g_{ij} + G_{ij} + \varepsilon_i \varepsilon_j H_{ij} & \text{if } i < j \end{cases}$$

we can then infer that

$$L = \sum_{i=1}^{n} m_{ii}^\varepsilon (\alpha_i \beta_i)^2 + 2 \sum_{i<j} m_{ij}^\varepsilon \varepsilon_i \varepsilon_j \alpha_i \alpha_j \beta_i \beta_j + \sum_{i<j} G_{ij} (\alpha_i \beta_j - \varepsilon_i \varepsilon_j \alpha_j \beta_i)^2 . \quad (10)$$

Step 1. We first discuss the necessary part. To get the Baker-Ericksen inequalities, i.e. $G_{ab} \geq 0$ for $1 \leq a < b \leq n$, choose $\alpha_i = 0$ if $i \neq a$, $\alpha_a = 1$ and $\beta_i = 0$ if $i \neq b$, $\beta_b = 1$. To obtain the copositivity of M^ε, it suffices to choose, given $x \in \mathbb{R}^n$ with $x_i \geq 0$, $\alpha_i = \sqrt{x_i}$ and $\beta_i = \varepsilon_i \sqrt{x_i}$ to get

$$L = \sum_{i=1}^{n} m_{ii}^\varepsilon (x_i)^2 + 2 \sum_{i<j} m_{ij}^\varepsilon x_i x_j \geq 0$$

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which is the claimed result.

Step 2. We now discuss the sufficiency part. We wish to show that Legendre-Hadamard condition in its form (10) is valid if M^ε is copositive and $G_{ij} \geq 0$. It is enough, given $\alpha, \beta \in \mathbb{R}^n$, to choose, for every $1 \leq i \leq n$, $\varepsilon_i = \pm 1$ so that

$$x_i = \varepsilon_i \alpha_i \beta_i \geq 0$$

to get the result. ∎

Of course the above lemma is not entirely satisfactory in the sense that, for general dimension, there is no simple criterion to know if a given matrix is copositive or not. However when $n = 2$ or $n = 3$ the situation is simpler and we discuss it now (the case $n = 2$ is well known and elementary, the case $n = 3$ is Theorem 4 of Hadeler [12]).

Proposition 4 *Let $A = (a_{ij}) \in \mathbb{R}_s^{n \times n}$ be an $n \times n$ symmetric matrix.*
(i) If $n = 2$ then A is copositive if and only if

$$a_{11}, a_{22} \geq 0$$

$$\sqrt{a_{11} a_{22}} + a_{12} \geq 0.$$

The matrix is strictly copositive if the inequalities are strict.
(ii) If $n = 3$ then A is copositive if and only if

$$a_{ii} \geq 0, \ i = 1, 2, 3 \tag{11}$$

$$\sqrt{a_{ii} a_{jj}} + a_{ij} \geq 0, \ 1 \leq i < j \leq 3 \tag{12}$$

and at least one of the following conditions holds

$$a_{12} \sqrt{a_{33}} + a_{13} \sqrt{a_{22}} + a_{23} \sqrt{a_{11}} + \sqrt{a_{11} a_{22} a_{33}} \geq 0 \tag{13}$$

$$\det A \geq 0. \tag{14}$$

The matrix is strictly copositive if (11), (12) are strict inequalities and if (13) holds (not necessarily with strict inequality) or if (14) holds with strict inequality.

The combination of the preceding lemma and proposition leads to

Theorem 5 *Let*
$$f(F) = g(\lambda_1(F), \lambda_2(F), \lambda_3(F))$$
where $g \in C^2(\mathbb{R}_+^3)$ and g is symmetric. Then $f : \mathbb{R}_+^{3 \times 3} \to \mathbb{R}$ is rank one convex if and only if the following four sets of conditions hold for every $\lambda \in \mathbb{R}_+^3$

$$g_{ii} \geq 0, \ i = 1, 2, 3 \tag{15}$$

$$\frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i - \lambda_j} \geq 0, \ \lambda_i \neq \lambda_j, \ 1 \leq i < j \leq 3 \tag{16}$$

$$\sqrt{g_{ii} g_{jj}} + m_{ij}^\varepsilon \geq 0, \ 1 \leq i < j \leq 3 \tag{17}$$

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and either

$$m_{12}^\varepsilon \sqrt{g_{33}} + m_{13}^\varepsilon \sqrt{g_{22}} + m_{23}^\varepsilon \sqrt{g_{11}} + \sqrt{g_{11} g_{22} g_{33}} \geq 0 \tag{18}$$

or

$$\det M^\varepsilon \geq 0 \tag{19}$$

where $M^\varepsilon = \left(m_{ij}^\varepsilon \right)$ is symmetric and

$$m_{ij}^\varepsilon = \begin{cases} g_{ii} & \text{if } i = j \text{ or if } i < j \text{ and } \lambda_i = \lambda_j \\ \varepsilon_i \varepsilon_j g_{ij} + \frac{g_i - \varepsilon_i \varepsilon_j g_j}{\lambda_i - \varepsilon_i \varepsilon_j \lambda_j} & \text{if } i < j \text{ and } \lambda_i \neq \lambda_j \text{ or } \varepsilon_i \varepsilon_j \neq 1 \end{cases}$$

and for any choice of $\varepsilon_i \in \{\pm 1\}$.

Remark 6 *If we are interested in the strong ellipticity then the necessary and sufficient conditions read as follows: (15), (16) hold with strict inequalities and either (18) holds (not necessarily with strict inequality) or (19) holds with strict inequality.*

We conclude this article by giving some simpler sufficient conditions that turn out to be also the necessary ones in dimension 2.

Proposition 7 *Let*

$$f(F) = g\left(\lambda_1(F), ..., \lambda_n(F) \right)$$

where $g \in C^2\left(\mathbb{R}_+^n \right)$ and g is symmetric. Then $f : \mathbb{R}_+^{n \times n} \to \mathbb{R}$ is rank one convex if the following four conditions hold for every $\lambda \in \mathbb{R}_+^n$

$$g_{ii} \geq 0, \ i = 1, ..., n \tag{20}$$

$$\frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i - \lambda_j} \geq 0, \ \lambda_i \neq \lambda_j, \ 1 \leq i < j \leq n \tag{21}$$

$$\frac{\sqrt{g_{ii} g_{jj}}}{n - 1} + g_{ij} + \frac{g_i - g_j}{\lambda_i - \lambda_j} \geq 0, \ \lambda_i \neq \lambda_j, \ 1 \leq i < j \leq n \tag{22}$$

$$\frac{\sqrt{g_{ii} g_{jj}}}{n - 1} - g_{ij} + \frac{g_i + g_j}{\lambda_i + \lambda_j} \geq 0, \ 1 \leq i < j \leq n. \tag{23}$$

Furthermore when $n = 2$ the conditions are also necessary.

Remark 8 *One advantage of Proposition 7 over Lemma 2 or Theorem 5 is that there are much less conditions to verify. In theory there are $(3n - 1) n / 2$ inequalities to check but because of all the symmetries it is enough to verify only 4 of them (for example those with $i = 1$ and $j = 2$).*

Proof. We discuss only the case where all the λ_i are different (the case where some of them are equal is handled similarly by passing to the limit). Recall the Legendre-Hadamard condition

$$L = \sum_{i,j=1}^n g_{ij} \alpha_i \alpha_j \beta_i \beta_j + \sum_{i \neq j} G_{ij} \alpha_i^2 \beta_j^2 + \sum_{i \neq j} H_{ij} \alpha_i \alpha_j \beta_i \beta_j \geq 0$$

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where
$$G_{ij} = \frac{\lambda_i g_i - \lambda_j g_j}{\lambda_i^2 - \lambda_j^2}, \ H_{ij} = \frac{\lambda_j g_i - \lambda_i g_j}{\lambda_i^2 - \lambda_j^2}.$$

We next rewrite L in a different manner. We first let ε_{ij} to be either 1 or -1. An elementary computation gives

$$\begin{aligned} L \ = \ & \frac{1}{n-1} \sum_{i<j} \left(\sqrt{g_{ii}} \alpha_i \beta_i + \sqrt{g_{jj}} \varepsilon_{ij} \alpha_j \beta_j \right)^2 + \sum_{i<j} G_{ij} \left(\alpha_i \beta_j + \varepsilon_{ij} \alpha_j \beta_i \right)^2 \\ & -2 \sum_{i<j} \left[\frac{\sqrt{g_{ii} g_{jj}}}{n-1} - \varepsilon_{ij} g_{ij} + G_{ij} - \varepsilon_{ij} H_{ij} \right] \varepsilon_{ij} \alpha_i \alpha_j \beta_i \beta_j. \end{aligned}$$

Observing that
$$G_{ij} - \varepsilon_{ij} H_{ij} = \frac{g_i + \varepsilon_{ij} g_j}{\lambda_i + \varepsilon_{ij} \lambda_j}$$

we get

$$\begin{aligned} L = \sum_{i<j} & \left[\frac{\left(\sqrt{g_{ii}} \alpha_i \beta_i + \sqrt{g_{jj}} \varepsilon_{ij} \alpha_j \beta_j \right)^2}{n-1} + G_{ij} \left(\alpha_i \beta_j + \varepsilon_{ij} \alpha_j \beta_i \right)^2 \right] \\ & -2 \sum_{i<j} \left[\frac{\sqrt{g_{ii} g_{jj}}}{n-1} - \varepsilon_{ij} g_{ij} + \frac{g_i + \varepsilon_{ij} g_j}{\lambda_i + \varepsilon_{ij} \lambda_j} \right] \varepsilon_{ij} \alpha_i \alpha_j \beta_i \beta_j. \end{aligned} \tag{24}$$

The result follows easily from (24). Indeed let $F \in \mathbb{R}_+^{n \times n}$ be such that (20) to (23) are satisfied. We wish to show that Legendre-Hadamard condition in its form (24) is valid. It is enough, given $\alpha, \beta \in \mathbb{R}^n$, to choose, for every $1 \le i < j \le n$, $\varepsilon_{ij} = \pm 1$ so that

$$\varepsilon_{ij} \alpha_i \alpha_j \beta_i \beta_j \le 0.$$

Then in view of (20) to (24) we have the claimed result.

The fact that when $n = 2$ the conditions are also necessary follows from Lemma 2 and Proposition 4. ∎

Remark 9 *One should note that if we consider the same problem but without the restriction* $\det F > 0$ *then all the conditions of Lemma 2 and Theorem 5 are obviously still necessary but are not anymore sufficient. One needs to impose some conditions of the type* $g_i \ge 0$ *at* $\lambda_i = 0$. *This matter is discussed for the case* $n = 2$ *in [10].*

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