On the convexity of the function $C \mapsto f(\det C)$ on positive-definite matrices

Stephan Lehmich, Patrizio Neff and Johannes Lankeit
Lehrstuhl für Nichtlineare Analysis und Modellierung, Fakultät für Mathematik, Universität Duisburg-Essen, Germany

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Abstract
Let $n \geq 2$. We prove a condition on $f \in C^2(\mathbb{R}_+, \mathbb{R})$ for the convexity of $f \circ \det$ on $\mathbb{PSym}(n)$, namely that $f \circ \det$ is convex on $\mathbb{PSym}(n)$ if and only if
$$f''(s) + \frac{n-1}{ns} \cdot f'(s) \geq 0 \quad \text{and} \quad f'(s) \leq 0 \quad \forall s \in \mathbb{R}_+.$$ 

This generalizes the observation that $C \mapsto -\ln \det C$ is convex as a function of $C$.

Keywords
Convexity, elasticity, Neo-Hooke model, ODE, polyconvexity

1. Introduction
The question of how to choose physically reasonable strain energy functions in nonlinear elasticity has attracted much attention and is not yet completely solved. The major breakthrough came with John Ball's seminal contributions [1–3] introducing polyconvexity, in other words, convexity of the strain energy $W$ as a function of the arguments $(F, \text{Cof } F, \det F)$ (see also [8, 9]). Polyconvexity reconciles the physically reasonable growth condition $W(F) \to \infty$ as $\det F \to 0$ with the weak-lower-semicontinuity (quasiconvexity), which in return implies ellipticity. A very simple example of a polyconvex function is the uni-constant compressible Neo-Hooke model
$$W_{NH}(F) = \mu [(F^TF - I \mathbb{1}) - 2 \ln \det(F)]_+,$$ 

where $\mu > 0$ is the shear modulus. The strain energy is isotropic, frame-indifferent, polyconvex (convex as a function of $(F, \det F)$), stress-free in the reference configuration, and $W_{NH} \to \infty$ as $\det F \to 0$. It is well known that the latter requirement excludes from the outset that $F \mapsto W_{NH}(F)$ may be a convex function of $F$ [6]. However, rewriting $W_{NH}$ in terms of the Cauchy–Green deformation tensor $C = F^TF$, which gives
$$W_{NH}(F) = \tilde{W}_{NH}(C) = \mu [(C - I \mathbb{1}) - \ln \det C],$$ 

one may readily check that $C \mapsto \tilde{W}_{NH}(C)$ is a convex function of $C$, despite its singularity in the determinant as $\det C \to 0$. We surmise that convexity of the free energy with respect to $C$ (or the stretch tensor $U = \sqrt{C}$) is an additional, desirable feature of any free energy as it implies monotonicity of the stress–strain relation. In this short contribution we therefore investigate which functions $f \in C^2(\mathbb{R}_+, \mathbb{R})$ are such that $C \mapsto f(\det C)$ is...
convex as function of $C \in \mathbb{PSym}(n)$ and generalize the well-known result that $C \mapsto -\ln \det C$ is convex on the set of positive-definite symmetric matrices [4, 5, 10] by proving:

**Theorem 1.1.** (A Differential Inequality Characterization) Let $f \in C^2(\mathbb{R}_+, \mathbb{R})$. Then the function

$$f \circ \det : \mathbb{PSym}(n) \to \mathbb{R}, \ C \mapsto f(\det C)$$

is convex if and only if

$$f''(s) + \frac{n-1}{ns} \cdot f'(s) \geq 0 \quad \text{and} \quad f'(s) \leq 0 \quad \forall s \in \mathbb{R}_+. \quad (1)$$

**Proof.** This is an immediate consequence of Lemmas 1.5, 1.7 and 1.9. □

In the following we will reformulate the condition for convexity to obtain this result. We start with some preliminaries:

By $\mathbb{M}^{n \times n}$ we denote the set of all real $n \times n$ matrices; $\mathbb{Sym}(n)$ stands for the set of all real symmetric $n \times n$ matrices, and $\mathbb{PSym}(n)$ for the set of all real symmetric positive-definite $n \times n$ matrices.

**Lemma 1.2.** (Characterization of Convexity) Let $X$ be a normed space, $K \subseteq X$ open and convex, and $g \in C^2(K, \mathbb{R})$. Then

$$g \text{ convex } \iff D^2g(x).(z, z) \geq 0 \quad \forall x \in K, \ z \in \text{span}(K). \quad (2)$$

**Proof.** See [7, p.27] □

In particular we obtain

**Theorem 1.3.** (Condition for Convexity) For $g \in C^2(\mathbb{PSym}(n), \mathbb{R})$ we have

$$g \text{ convex } \iff D^2g(C).(H, H) \geq 0 \quad \forall C \in \mathbb{PSym}(n), \ H \in \mathbb{Sym}(n). \quad (3)$$

**Proof.** Let $K := \mathbb{PSym}(n)$ and $X := \mathbb{Sym}(n)$ in the previous lemma. $\mathbb{PSym}(n)$ is an open convex subset of the normed space $\mathbb{Sym}(n)$ (with operator norm): use the characterization $A \in \mathbb{PSym}(n) \iff \langle Ax, x \rangle > 0 \ \forall x \in \mathbb{R}^n \setminus \{0\}$, and for convexity also use the Cauchy–Schwarz inequality. Furthermore, $\text{span}(K) = \text{span}(\mathbb{PSym}(n)) = \mathbb{Sym}(n) = X$: the inclusion $\subseteq$ is obvious. For the other inclusion, write $A$ as a diagonal matrix (the corresponding transformation preserves positive-definiteness and symmetry) and show that this can be written as a linear combination of positive-definite symmetric matrices. □

By $\langle A, B \rangle = \text{tr}(AB^T)$ we denote the trace inner product of the matrices $A$ and $B$.

**Theorem 1.4.** (A Condition for Convexity)

Let $f \in C^2(\mathbb{R}_+, \mathbb{R})$. Then the function

$$g := f \circ \det : \mathbb{PSym}(n) \to \mathbb{R}, \ C \mapsto f(\det C)$$

is convex if and only if

$$\forall C \in \mathbb{PSym}(n) \ \forall H \in \mathbb{Sym}(n):$$

$$\left[ f''(\det C) \det C + f'(\det C) \right] (C^{-1}, H)^2 - f'(\det C) \langle HC^{-1}, C^{-1}H \rangle \geq 0. \quad (4)$$

**Proof.** Because $f \in C^2$, and $\det \in C^\infty$, also $g \in C^2$. It remains to be shown that

$$D^2g(C).(H, H) = \det C \cdot \left\{ \left[ f''(\det C) \cdot \det C + f'(\det C) \right] \cdot (C^{-1}, H)^2 - f'(\det C) \cdot \langle HC^{-1}, C^{-1}H \rangle \right\}$$
for $C \in \mathbb{P} \text{Sym}(n)$ and $H \in \text{Sym}(n)$. The claim follows by Theorem 1.3. Because $\det$ is infinitely often differentiable on $M_{n \times n}$ and $D \det(A)H = \langle \text{Adj } A^T, H \rangle$ (cf. [6]), where $\text{Adj } A$ denotes the adjugate matrix of $A$, for invertible $C$ and symmetric $H$ we have $D \det(C)H = \det(C(C^{-1}, H))$, and hence obtain by the chain rule

$$Dg(C).H = Df(\det(C))D(\det(C)).H = f'(\det(C)) \cdot \det(C) \cdot \langle C^{-1}, H \rangle,$$

and therefore, by chain rule and the fact that $D[C^{-1}].H = -C^{-1}HC^{-1}$,

$$D^2g(C).(H,H) = f''(\det(C)) \cdot (\det(C))^2 \cdot \langle C^{-1}, H \rangle^2 + f'(\det(C)) \cdot \det(C) \cdot \langle C^{-1}, H \rangle^2 + f'(\det(C)) \cdot \det(C) \cdot \langle -(C^{-1}HC^{-1}), H \rangle$$

$$= f''(\det(C)) \cdot \det(C^2) \cdot \langle C^{-1}, H \rangle^2 + f'(\det(C)) \cdot \det(C) \cdot \langle C^{-1}, H \rangle^2 + f'(\det(C)) \cdot \det(C) \cdot \langle HC^{-1}, C^{-1}H \rangle. \quad (5)$$

**Lemma 1.5.** The inequality $f'(s) \leq 0 \quad \forall s \in \mathbb{R}_+$ is necessary for inequality (4).

**Proof.** Assume $s \in \mathbb{R}_+$ satisfying $f'(s) > 0$. Let $C = \text{diag}(\sqrt{s}, \sqrt{s}, 1, \ldots, 1) \in \mathbb{P} \text{Sym}(n)$ and $H = \text{diag}(1, -1, 0, \ldots, 0) \in \text{Sym}(n)$. Then $\det(C) = s$, $\langle C^{-1}, H \rangle = \frac{1}{\sqrt{s}} - \frac{1}{\sqrt{s}} = 0$ and

$$\langle HC^{-1}, C^{-1}H \rangle = \langle \text{diag}(\frac{1}{\sqrt{s}}, -\frac{1}{\sqrt{s}}, 0, \ldots, 0), \text{diag}(\frac{1}{\sqrt{s}}, -\frac{1}{\sqrt{s}}, 0, \ldots, 0) \rangle = \frac{2}{s}. \quad \text{Together with inequality (4) we obtain}$$

$$-\frac{2}{s}f'(s) \geq 0, \quad \text{a contradiction to} \quad f'(s) > 0.$$

**Lemma 1.6.** Inequality (4) holds if and only if

$$\forall H \in \text{Sym}(n) \quad \forall D^{-1} = \text{diag}(d_1, \ldots, d_n),$$

where $d_1, \ldots, d_n \in \mathbb{R}_+$ and $s^{-1} := \det(D^{-1}) = d_1 \cdot \ldots \cdot d_n \in \mathbb{R}_+$:

$$\left(f''(s) + \frac{f'(s)}{s}\right) \langle D^{-1}, H \rangle^2 = \frac{f'(s)}{s} \langle D^{-1}H, HD^{-1} \rangle \geq 0. \quad (6)$$

**Proof.** In inequality (4) consider an arbitrary $C \in \mathbb{P} \text{Sym}(n)$. Then there is an orthogonal matrix $Q$, such that $C = QDQ^T \Leftrightarrow C^{-1} = QD^{-1}Q^T$, where $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$ and $\lambda_i$ are positive. By the properties of the scalar product of matrices we have

$$\langle C^{-1}, H \rangle = \langle QDQ^T, H \rangle = \langle QD^{-1}Q^T, HQ \rangle = \langle QD^{-1}, Q^THQ \rangle.$$  

For $H \in \text{Sym}(n)$ let $\widetilde{H} := Q^THQ$ and note that $H$ varies over the whole of $\text{Sym}(n)$ if and only if $\widetilde{H}$ does. Analogously,

$$\langle HC^{-1}, C^{-1}H \rangle = \langle HQD^{-1}Q^T, QD^{-1}Q^TH \rangle = \langle \widetilde{H}D^{-1}, D^{-1}\widetilde{H} \rangle = \langle D^{-1}\widetilde{H}, \widetilde{H}D^{-1} \rangle.$$  

Denote $d_i := \lambda_i^{-1}$ and $s := \det(C) = \det(D) = \prod_{i=1}^{n} \lambda_i$, and divide inequality (4) by $s > 0$ to obtain condition (6).

**Lemma 1.7.** Let $f \in C^2(\mathbb{R}_+, \mathbb{R})$ and $f \circ \det$ be convex on $\mathbb{P} \text{Sym}(n)$. Then $f''(s) \geq -\frac{n-1}{n} \frac{f'(s)}{s} \forall s \in \mathbb{R}_+$.

**Proof.** According to Theorem 1.4 and Lemma 1.6, condition (6) holds for all $H \in \text{Sym}(n)$ and $D^{-1} = \text{diag}(d_1, \ldots, d_n)$. Let $s \in \mathbb{R}_+, k \in \mathbb{R} \setminus \{0\}$ and $H = k \cdot D^{-1}$, as well as $D^{-1} = \text{diag}(s^{-1}e_1, \ldots, s^{-1}e_n)$.

$$0 \leq k^2 \left( \left( f''(s) + \frac{f'(s)}{s}\right) \langle D^{-1}, D^{-1} \rangle^2 - \frac{f'(s)}{s} \langle (D^{-1})^2, (D^{-1})^2 \rangle \right)$$

$$= k^2 \left( \left( f''(s) + \frac{f'(s)}{s}\right) \langle \text{tr}(D^{-1})^2, \text{tr}(D^{-1})^2 \rangle - \frac{f'(s)}{s} \cdot \text{tr}(D^{-1})^4 \right)$$

$$= k^2 \left( \left( f''(s) + \frac{f'(s)}{s}\right) \langle ns^{-2/n}, ns^{-2/n} \rangle - \frac{f'(s)}{s} \cdot ns^{-4/n} \right) = nk^2s^{-4/n} \left( nf''(s) + (n-1)\frac{f'(s)}{s} \right).$$

\[\square\]
For any matrix $A$ let $\text{diag} A$ be the matrix obtained from $A$ by setting all non-diagonal entries to zero. Let $\text{diag}_{3 \times 3}$ be the set of all $3 \times 3$ diagonal matrices.

**Lemma 1.8.** For all $P \in \text{diag}_{3 \times 3}$ with non-negative entries only, and all $A \in M^{n \times n}$, the following holds:

\[
\langle P, A \rangle = \langle P, \text{diag} A \rangle := \sigma(P, A),
\]

(7)

\[
\langle PA, AP \rangle \geq \langle P \text{ diag } A, \text{ diag } A P \rangle := \tilde{\sigma}(P, A),
\]

(8)

\[
\sigma^2(P, A) \leq n \cdot \tilde{\sigma}(P, A).
\]

(9)

**Proof.** Let $P = \text{diag}(p_1, \ldots, p_n)$, $A = (a_{ij})$, and calculate $\langle P, A \rangle = \sum_{i=1}^n p_i a_{ii} = \langle P, \text{ diag } A \rangle$. Hence equation (7) holds. Direct calculation of $PA$ and $PA^T$ yields

\[
\langle PA, AP \rangle = \text{tr}(PA^T) = \sum_{i=1}^n p_i^2 a_{ii}^2 + \sum_{i=1}^n \sum_{k \neq i}^n p_i p_k a_{ik}^2 \geq \langle P \text{ diag } A, \text{ diag } A P \rangle,
\]

in other words, equation (8). For all $P \in \text{diag}_{3 \times 3}$ and $A \in M^{n \times n}$, we have $\sigma^2(P, A) \leq n \cdot \tilde{\sigma}(P, A)$. To see this, note that $P$ and $\text{ diag } A$ commute: $\tilde{\sigma}(P, A) = (P \text{ diag } A, P \text{ diag } A) = \|P \text{ diag } A\|^2$ holds. By the Cauchy–Schwarz inequality this immediately implies

\[
\sigma^2(P, A) = \langle P, \text{ diag } A \rangle^2 = \langle P \text{ diag } A, \mathbb{I} \rangle^2 \leq \|P \text{ diag } A\|^2 \cdot \|\mathbb{I}\|^2 = n \cdot \tilde{\sigma}(P, A).
\]

\[\square\]

**Lemma 1.9.** Inequalities (1) are sufficient for $f \circ \text{ det}$ to be convex.

**Proof.** We will show inequality (6). To this end, let $H \in \text{ Sym}(n)$ and $D^{-1} = \text{ diag}(d_1, \ldots, d_n)$, where $d_1, \ldots, d_n \in \mathbb{R}^+$ and $s := (d_1 \cdots d_n)^{-1} = \text{ det } D$ arbitrary. Then $P := D^{-1}$ and $A := H$ satisfy all assumptions of the previous lemma. Using the notation from Lemma 1.8, we can, without loss of generality, assume $\sigma(D^{-1}, H) = 0$, because otherwise condition (6) becomes trivial by the assumption $f'' \leq 0$. We denote $\sigma = \sigma(D^{-1}, H)$ and $\tilde{\sigma} = \tilde{\sigma}(D^{-1}, H) \leq (D^{-1}H, HD^{-1})$ by inequality (8). Using $f''(s) + \frac{n-1}{n} f'(s) \geq 0$, by inequality (1) and $1 - \frac{\tilde{\sigma}}{\sigma} \leq \frac{n-1}{n}$, we obtain condition (6) from

\[
\left( f''(s) + \frac{f'(s)}{s} \right) (D^{-1}, H)^2 - \frac{f'(s)}{s} (D^{-1}H, HD^{-1}) \geq \left( f''(s) + \frac{f'(s)}{s} \right) \cdot \sigma^2 - \frac{f'(s)}{s} \cdot \tilde{\sigma}
\]

\[
= \sigma^2 \cdot \left[ f''(s) + \frac{f'(s)}{s} \cdot \left( 1 - \frac{\tilde{\sigma}}{\sigma^2} \right) \right] \geq \sigma^2 \cdot \left( f''(s) + \frac{n-1}{n} \cdot \frac{f'(s)}{s} \right) \geq 0.
\]

\[\square\]

2. Solutions to the differential inequalities

In this section we are interested in the possible shape of the functions that satisfy inequality (1). To make calculations and figures more concrete, we restrict ourselves to the case $n = 3$.

**Lemma 2.1.** (LINEAR ODE) The linear initial value problem

\[
Ly := y' + g(x)y = 0, \quad y(\xi) = \eta
\]

(LIVP)

on $J = \mathbb{R}_+$ and where $g(x) = \frac{2}{3x}$ has one and only one solution.

To find solutions to $Lf'' \geq 0$ under the additional constraint $y = f' \leq 0$ (which is equivalent to $\eta \leq 0$ because $f'' \equiv 0$ is a solution) we consider the ‘limiting case’:

**Lemma 2.2.** (LIMITING CASE FOR INEQUALITY (1)) The solutions to

\[
f''_{\text{lim}}(s) + \frac{2}{3s} \cdot f'_{\text{lim}}(s) = 0 \quad \text{and} \quad f'_{\text{lim}}(s) \leq 0 \quad \forall s \in \mathbb{R}_+
\]

are given by $f_{\text{lim}}: \mathbb{R}_+ \to \mathbb{R}, \ s \mapsto c \cdot s^{1/3} + d$, where $c \leq 0, \ d \in \mathbb{R}$. 

**Proof.** Separation of variables gives the unique solution of equation (LIVP) for $\xi > 0 \geq \eta$:

$$y_{\text{lim}}(x) = \eta \cdot \exp \left( - \int_{\xi}^{x} \frac{2}{3} \, dt \right) = \eta \cdot \exp \left( - \frac{2}{3} \ln \frac{x}{\xi} \right) = \eta \xi^{2/3} \cdot x^{-2/3}. \tag{10}$$

Because $\eta \xi^{2/3} \leq 0$, we have $y_{\text{lim}} \leq 0$, hence inequality (1). The claim follows by integration of $f'' = y_{\text{lim}}$ with $c := 3\eta \xi^{2/3}$ and constant $d$. \hfill $\square$

If we consider an interval adjacent to $\xi$ on the left hand side, in other words, $\tilde{J} : = [\xi - \alpha, \xi]$, the conditions for a function $y$ to be a sub- (or super-) solution to $y' = f(x, y)$, $y(\xi) = \eta$ are

$$y' \left\{ \begin{array}{c} > \\ \geq \end{array} \right. \left\{ \begin{array}{c} > \\ \geq \end{array} \right. \left\{ \begin{array}{c} \geq \\ \geq \end{array} \right. F(\xi, v) \text{ in } \tilde{J}, \quad v(\xi) \leq \eta \quad \text{(or } w' \left\{ \begin{array}{c} < \\ \leq \end{array} \right. \left\{ \begin{array}{c} < \\ \leq \end{array} \right. F(\xi, w) \text{ in } \tilde{J}, \quad w(\xi) \geq \eta \text{ respectively}) \right.,$$

where (see equation (LIVP)) $F_{2/3}(x, y) := -\frac{2}{3x} \cdot y \in C^\infty(\mathbb{R} \times [0, \infty))$ yields

**Lemma 2.3.** Let $y$ be differentiable in $\mathbb{R}_+$, $\xi > 0 \geq \eta$. Then

$$y' \left\{ \begin{array}{c} > \\ \geq \end{array} \right. F_{2/3}(x, y), \quad y(\xi) \geq \eta \implies y(x) \left\{ \begin{array}{c} > \\ \geq \end{array} \right. y_{\text{lim}}(x) = \eta \xi^{2/3} \cdot x^{-2/3} \text{ on } \left\{ \begin{array}{c} (\xi, \infty) \\ [\xi, \infty) \end{array} \right..$$

Analogously:

$$y' \left\{ \begin{array}{c} > \\ \geq \end{array} \right. F_{2/3}(x, y), \quad y(\xi) \leq \eta \implies y(x) \left\{ \begin{array}{c} < \\ \leq \end{array} \right. y_{\text{lim}}(x) \text{ on } \left\{ \begin{array}{c} (0, \xi) \\ (0, \xi) \end{array} \right..$$

By these considerations, we obtain information on the qualitative shape of solutions to inequality (1) (at first discussing the shape of $y = f'$, see Figure 1). Note that to fulfill $y \leq 0$, in Lemma 2.3 $0 \geq y(\xi) \geq \eta$ must also be satisfied. For $\eta = 0$, $y_{\text{lim}} = 0$ is the unique solution and intersects $y$ in $\xi$, $(0 \geq y(\xi) \geq 0)$. For $0 \geq y(\xi) > \eta$, $y$ and $y_{\text{lim}}$ with initial value $y_{\text{lim}}(\xi) = y(\xi)$ intersect in $\xi$. Hence we can consider $y(\xi) = \eta = y_{\text{lim}}(\xi)$ only. Then

$$y' \left\{ \begin{array}{c} > \\ \geq \end{array} \right. -\frac{2}{3x} \cdot y = F_{2/3}(x, y), \quad y(\xi) = \eta$$

implies

$$y \left\{ \begin{array}{c} > \\ \geq \end{array} \right. y_{\text{lim}} \text{ on } \left\{ \begin{array}{c} (\xi, \infty) \\ [\xi, \infty) \end{array} \right. \text{ and } y \left\{ \begin{array}{c} < \\ \leq \end{array} \right. \left\{ \begin{array}{c} (0, \xi) \\ (0, \xi) \end{array} \right..$$

Additionally, the graphs of solutions $y_{\text{lim}}$ contain the points $(1, \eta \xi^{2/3})$. Hence there is no need to consider initial values different from $y(1) = \eta = y_{\text{lim}}(1)$ for $\eta \leq 0$.

Therefore all (derivatives $y$ of) solutions to equation (1) qualitatively have the shape of the dashed line in Figure 1 ($y \leq 0$, $y' = f'' \geq 0$; furthermore, $f$ and $f_{\text{lim}}$ have the same slope in 1). In $(0, 1)$, however, $f$ decreases more rapidly than $f_{\text{lim}}$; in $(1, \infty)$, less rapidly.

The question now is: are there other solutions to equation (1)? Note that for example the attempt to find a solution by solving $y' = \tilde{F}(x, y) := F_{2/3}(x, y) + \varepsilon$ for some positive $\varepsilon$ leads to solutions that satisfy $f'' \leq 0$ in a bounded neighbourhood of $\xi$ only and not on the whole of $\mathbb{R}_+$. However, $\tilde{F}(x, y) := F_{2/3}(x, y) = -\frac{2}{3x(y + a)} = -\frac{3a + 2}{3x}y$ for $a \geq 0$ gives $y_a(x) = \eta \cdot \exp \left( -\int_{1}^{x} \frac{3a + 2}{3t} \, dt \right) = \eta \cdot x^{-\left(\frac{2}{3} + a\right)}$ as solution to

$$y'_a = -\frac{3a + 2}{3x}y_a \quad \text{and} \quad y_a(1) = \eta \leq 0$$

and hence we obtain the following family of solutions to inequality (1):

**Lemma 2.4.** (FAMILY OF SOLUTIONS) For arbitrary $c \leq 0$, $d \in \mathbb{R}$, $a \in [0, \infty)$, the family of functions that is defined on $\mathbb{R}_+$ by

$$f_a(s) := \begin{cases} d + c \cdot s^{\frac{1}{3} - a} & , \text{ for } a \in [0, 1/3) \\ d + c \cdot \ln s & , \text{ for } a = 1/3 \\ d - c \cdot s^{\frac{1}{3} - a} & , \text{ for } a \in (1/3, \infty) \end{cases}$$

has the property that $f_a \circ \det : \text{PSym}(3) \rightarrow \mathbb{R}$, $C \mapsto f_a(\det C)$ is convex.
Figure 1. The shape of $y = f'$ for solutions $f$ of inequality (1).

Figure 2. Qualitative shape of solutions to inequality (1).

Remark 2.5. Although this condition is not necessary for the convexity of $f \circ \text{det}$, at least qualitatively all solutions to inequality (1) have the shape indicated in the graph in Figure 2 (as we discussed in this section).

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