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SOME NUMERICAL METHODS FOR THE STUDY OF THE CONVEXITY NOTIONS ARISING IN THE CALCULUS OF VARIATIONS (*)

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Résumé — *Nous proposons des méthodes numenques pour la détermmation de la convexıté, polyconvexıté, quasıconvexıté et la convexıté de rang un d'une fonctıon Ces notıons sont d'ımportance fondamentale pour les problèmes vectorıels du calcul des varıatıons*

Abstract — *We propose numerıcal schemes to determıne whether a gıven functıon ıs convex, polyconvex, quasıconvex and rank one convex These notıons are of fundamental ımportance ın the vectorıal problems of the calculus of varıatıons*

Key words : calculus of varıatıons, convexıty, polyconvexıty, quasıconvexıty, rank one convexıty

1. INTRODUCTION

One of the most important problems in the calculus of variations deals with the integral

$$I(u) = \int_\Omega f(\nabla u(x))\, dx \tag{1}$$

where
1. $\Omega \subset \mathbb{R}^n$ is a bounded open set,
2. $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ belongs to a Sobolev space,
3. $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ is a continuous function.

Usually one wants to minimize (1) subject to some constraints, e.g. certain boundary conditions, isoperimetric constraints, etc... The only general method to deal with these problems consists in proving the sequential weak lower semicontinuity of $I(u)$. When $m = 1$ or $n = 1$, this property is equivalent to the convexity of f. However, when $m, n > 1$, it is equivalent to the so called quasiconvexity of f, a notion introduced by Morrey [23].

DEFINITION 1.1: *A continuous function* $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ *is* quasiconvex *if*

$$\int_\Omega [f(\xi + \nabla\varphi(x)) - f(\xi)]\, dx \geq 0$$

for every $\xi \in \mathbb{R}^{m \times n}$, *for every bounded open subset* Ω *of* $\mathbb{R}^n$ *and every* $\varphi \in W_0^{1,\infty}(\Omega ; \mathbb{R}^m)$ *(i.e.* $\varphi : \Omega \to \mathbb{R}^m$ *is continuous, has uniformly bounded gradient, and* $\varphi = 0$ *on* $\partial\Omega$.*)*

However, except in a few cases, this is analytically an almost intractable notion. One is therefore led to introduce some weaker and stronger notions, namely rank one convexity and polyconvexity.

DEFINITION 1.2: *A function* $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ *is* rank one convex *if*

$$f(\lambda\xi + (1-\lambda)\eta) \leq \lambda f(\xi) + (1-\lambda) f(\eta)$$

whenever $\lambda \in [0, 1], \xi, \eta \in \mathbb{R}^{m \times n}$ *with* $\mathbf{rank}\,(\xi - \eta) \leq 1$.

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DEFINITION 1.3: *A function* $f\colon \mathbb{R}^{m\times n} \to \mathbb{R}$ *is* polyconvex *if there exists a convex function* g *such that*

$$f(\xi) = g(\xi, \text{minors of } \xi)\,.$$

More precisely, if $m = n = 2$, then $g : \mathbb{R}^{2\times 2} \times \mathbb{R} \to \mathbb{R}$ is convex and

$$f(\xi) = g(\xi, \det \xi)\,.$$

Remark 1.1. The general relationship between these notions is as follows:

$$f \text{ convex} \Rightarrow f \text{ polyconvex} \Rightarrow f \text{ quasiconvex} \Rightarrow f \text{ rank one convex}\,.$$

For more details see Ball [4] and Dacorogna [12]. The converse to each of the above implications is false, however. For example, when $m = n = 2$, $f(\xi) = \det \xi$ is polyconvex but not convex. The existence of a rank one convex function that is not quasiconvex when $n \geqslant 2$, $m \geqslant 3$ was proved by Sverak [30]. In the case $m = 2$, however, it is still an open question to determine whether

$$f \text{ rank one convex} \Rightarrow \text{f quasiconvex}\,. \tag{2}$$

In view of the difficulties involved in checking analytically these notions, we present in this paper some numerical schemes to verify if a given function has the desired convexity property. In particular we are interested in comparing, in the case $m = n = 2$, rank one convexity and quasiconvexity, checking numerically for their equivalence. We have studied a great many examples in the case $n = 2$ and $m = 2$ or 3. The conclusions of our extensive computations are the following.

1. The numerical results are in complete agreement with all the known analytical results. In particular, when $m = 3$ and $n = 2$, we had no difficulty checking numerically that Sverak's function is rank one convex but not quasiconvex.
2. In all examples we tested, when $m = n = 2$, quasiconvexity and rank one convexity turned out to be equivalent, thereby suggesting that (2) is true in this case. This is in agreement with earlier numerical experiments [13, 18].

Finally, it should be noted that numerical computations on these questions and related ones have been treated by many authors. See, for example, Dacorogna-Douchet-Gangbo-Rappaz [13], Dacorogna-Haeberly [14], Brighi-Chipot [6], Chipot [7], Chipot-Collins [8], Chipot-Lécuyer [9], Collins-Kinderlehrer-Luskin [10], Collins-Luskin [11] and Gremaud [18]. Unfortunately, besides [14], only [13] and [18] actually contain numerical data with which to compare our results.

This paper is organized as follows: In Section 2 we discuss several families of functions. These families have been studied extensively and many analytical results concerning their convexity, polyconvexity, and rank one convexity properties have been proved. In contrast, we have almost no information about their quasiconvexity. In Section 3 we show how the problem of determining whether a given function is convex, polyconvex, quasiconvex, or rank one convex reduces to solving a, possibly constrained, optimization problem. In Section 4 we introduce two general schemes for checking the convexity properties of a function such as those described in Section 2. In Section 5, we discuss the algorithms we used to solve the optimization problem. In Section 6 we present our numerical results for the families of functions introduced in Section 2. Finally, in Section 7 we discuss further numerical investigations in the case $n = 2$, $m = 2$ or 3.

Notation. For $\xi, \eta \in \mathbb{R}^{m\times n}$ we write $\langle \xi ; \eta \rangle$ for the standard inner product on $\mathbb{R}^{m\times n}$, namely

$$\langle \xi ; \eta \rangle = \mathbf{tr}\,(\xi^T \eta) = \sum_{i=1}^{m} \sum_{j=1}^{n} \xi_{ij}\,\eta_{ij}\,,$$

and we write

$$|\xi| = \sqrt{\langle \xi ; \xi \rangle}\,.$$

For $a \in \mathbb{R}^m$, $b \in \mathbb{R}^n$ we let $a \otimes b \in \mathbb{R}^{m \times n}$ denote the rank one matrix

$$\begin{pmatrix} a_1 b_1 & \dots & a_1 b_n \\ \vdots & \dots & \vdots \\ a_m b_1 & \dots & a_m b_n \end{pmatrix}.$$

Note that all $m \times n$ matrices of rank one are of the form $a \otimes b$ for suitable a and b, although this representation is not unique.

When $m = n$, we let $\mathbb{R}_+^{n \times n}$ and $\mathbb{R}_-^{n \times n}$ denote those $n \times n$ matrices ξ with $\det \xi > 0$, respectively $\det \xi < 0$.

For $\xi \in \mathbb{R}^{3 \times 2}$ we write

$$\operatorname{adj} \xi = (\xi_{21} \xi_{32} - \xi_{22} \xi_{31}, -\xi_{11} \xi_{32} + \xi_{12} \xi_{31}, \xi_{11} \xi_{22} - \xi_{12} \xi_{21}) \in \mathbb{R}^3$$

for the vector of minors of ξ.

Finally, we will often abuse the notation and think of a matrix $\xi \in \mathbb{R}^{m \times n}$ as a vector in $\mathbb{R}^{mn}$, and conversely. By convention, the vector corresponding to the matrix

$$\xi = \begin{pmatrix} \xi_{11} & \dots & \xi_{1n} \\ \vdots & \dots & \vdots \\ \xi_{m1} & \dots & \xi_{mn} \end{pmatrix}$$

is given by

$$(\xi_{11}, \dots, \xi_{1n}, \dots, \xi_{m1}, \dots, \xi_{mn}).$$

2. FAMILIES OF EXAMPLES

We present several families of functions that have been studied extensively in the literature, and we recall all the known results about their convexity properties.

Example 1. Let $m = n = 2$, $\gamma \in \mathbb{R}$, $\alpha \geq 1$, and

$$f_\gamma(\xi) = |\xi|^{2\alpha}(|\xi|^2 - \gamma \det \xi).$$

The case $\alpha = 1$ has been studied by Dacorogna-Marcellini [16] and Alibert-Dacorogna [1] (see also Hartwig [19], Iwaniec-Lutoborski [20]). They proved that

$$\begin{cases} f_\gamma \text{ is convex} \Leftrightarrow |\gamma| \leq \frac{4}{3}\sqrt{2} \\ f_\gamma \text{ is polyconvex} \Leftrightarrow |\gamma| \leq 2 \\ f_\gamma \text{ is quasiconvex} \Leftrightarrow |\gamma| \leq 2 + \epsilon, \text{ where } \epsilon > 0, \text{ but not explicitly known} \\ f_\gamma \text{ is rank one convex} \Leftrightarrow |\gamma| \leq \dfrac{4}{\sqrt{3}} \end{cases}$$

When $\alpha > 1$, it has been established by Dacorogna-Douchet-Gangbo-Rappaz [13] that

$$f_\gamma \text{ is rank one convex} \Leftrightarrow |\gamma| \leq \gamma_r = \begin{cases} \gamma_1 & \text{if } \alpha \in \left[1, \dfrac{9 + 5\sqrt{5}}{4}\right), \\ \gamma_2 & \text{if } \alpha \geq \dfrac{9 + 5\sqrt{5}}{4} \end{cases}$$

where

$$\gamma_1 = \left(1 + \frac{1}{\alpha}\right) \min_{t>0} \left\{ \frac{t^4 + 2(\alpha+1)t^2 + 2\alpha + 1}{3t^3 + (2\alpha+1)t} \right\}$$

and

$$\gamma_2 = 1 + \sqrt{1 - \frac{1}{2\alpha} - \frac{1}{2\alpha^2}}$$

Observe that f_γ is smooth and homogeneous of degree $2(\alpha+1)$.

Example 2. Let $m = n = 2$, $\gamma \geq 0$, $\alpha \geq \frac{1}{4}$, and

$$f_\gamma(\xi) = |\xi|^{4\alpha} - 2^{2\alpha-1}\gamma((\det \xi)^2)^\alpha .$$

Ball and Murat [5] have shown that if $\frac{1}{4} < \alpha < 1$ then

$$\begin{aligned} f_\gamma \text{ is convex} &\Leftrightarrow f_\gamma \text{ is polyconvex} \\ &\Leftrightarrow f_\gamma \text{ is quasiconvex} \\ &\Leftrightarrow f_\gamma \text{ is rank one convex} \\ &\Leftrightarrow \gamma = 0 . \end{aligned}$$

If $\alpha = 1$, it is easy to see that

$$\begin{aligned} f_\gamma \text{ is convex} &\Leftrightarrow f_\gamma \text{ is polyconvex} \\ &\Leftrightarrow f_\gamma \text{ is quasiconvex} \\ &\Leftrightarrow f_\gamma \text{ is rank one convex} \\ &\Leftrightarrow \gamma \leq 1 . \end{aligned}$$

If $\alpha > 1$, it has been established by Dacorogna-Douchet-Gangbo-Rappaz [13] that

$$f_\gamma \text{ is rank one convex} \Leftrightarrow \gamma \leq \gamma_r = \begin{cases} \gamma_1 & \text{if } 1 < \alpha < 1 + \frac{1}{\sqrt{2}} \\ \gamma_2 & \text{if } \alpha \geq 1 + \frac{1}{\sqrt{2}} \end{cases}$$

where

$$\gamma_1 = \frac{2(2\alpha + (2\alpha-1)z)}{(2\alpha-1)(1-z)(1-z^2)^{\alpha-1}}$$

$$\gamma_2 = \frac{\dfrac{2(2\alpha-1)}{4\alpha-1}}{\left(1 - \dfrac{\alpha}{(2\alpha-1)^2}\right)^{2(\alpha-1)}}$$

with

$$z = \frac{-(4\alpha^2 - 1) + \sqrt{(4\alpha^2 - 1)^2 - 8(2\alpha - 1)(\alpha - 1)(4\alpha - 1)}}{4(2\alpha - 1)(\alpha - 1)}$$

Observe that for $\gamma \leqslant 0$, f_γ is obviously polyconvex, and hence quasiconvex and rank one convex. Furthermore f_γ is smooth and homogeneous of degree 4α.

Example 3. Let $m = n = 2$, and let $M \in \mathbb{R}^{4 \times 4}$ be a symmetric matrix whose eigenvalues are $\mu_1 \leqslant \mu_2 \leqslant \mu_3 \leqslant \mu_4$. Let $\gamma \geqslant 0$, and, identifying $\mathbb{R}^{2 \times 2}$ with $\mathbb{R}^4$, let

$$f_\gamma(\xi) = \begin{cases} |\xi| + \gamma \dfrac{\langle M\xi ; \xi \rangle}{|\xi|} & \text{if } \xi \neq 0 \\ 0 & \text{if } \xi = 0 \end{cases}$$

Dacorogna and Haeberly [15] proved that

$$f_\gamma \text{ is convex} \Leftrightarrow f_\gamma, \text{ is polyconvex} \Leftrightarrow \gamma \leqslant \gamma_c = \begin{cases} \dfrac{1}{\mu_4 - 2\mu_1} & \text{if } \mu_4 - 2\mu_1 > 0 \\ +\infty & \text{if } \mu_4 - 2\mu_1 \leqslant 0 \end{cases}$$

Under some restrictions on the eigenvectors of M (see [15]), we have

$$f_\gamma \text{ is rank one convex} \Leftrightarrow \gamma \leqslant \gamma_r = \begin{cases} \min\left\{\dfrac{1}{\gamma_1}, \dfrac{1}{\gamma_2}\right\} & \text{if } \gamma_1 > 0 \text{ and } \gamma_2 > 0 \\ \dfrac{1}{\gamma_2} & \text{if } \gamma_1 \leqslant 0 \text{ and } \gamma_2 > 0 \\ \dfrac{1}{\gamma_1} & \text{if } \gamma_1 > 0 \text{ and } \gamma_2 \leqslant 0 \\ +\infty & \text{if } \gamma_1 \leqslant 0 \text{ and } \gamma_2 \leqslant 0 \end{cases}$$

where

$$\gamma_1 = \frac{\mu_4 + \mu_3}{2} - 2\mu_1 \quad \text{and} \quad \gamma_2 = \mu_4 - (\mu_1 + \mu_2) .$$

Observe that f_γ is smooth on $\mathbb{R}^{2 \times 2} - \{0\}$ and homogeneous of degree 1.

Example 4. Let $m = 3$, $n = 2$ and let $P : \mathbb{R}^{3 \times 2} \to \mathbb{R}^{3 \times 2}$ be defined as

$$P\begin{pmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \\ \xi_{31} & \xi_{32} \end{pmatrix} = \begin{pmatrix} \xi_{11} & 0 \\ 0 & \xi_{22} \\ \dfrac{\xi_{31} + \xi_{32}}{2} & \dfrac{\xi_{31} + \xi_{32}}{2} \end{pmatrix} .$$

Let g be the function defined on the image of P and given by

$$g\begin{pmatrix} r & 0 \\ 0 & s \\ t & t \end{pmatrix} = -rst .$$

Let $\gamma > 0$ and $\alpha > 0$, and consider the function

$$f_\gamma = |\xi - P\xi|^2 + \gamma(g(P\xi) + \alpha(|\xi|^2 + |\xi|^4)) .$$

This is essentially the counterexample of Sverak [30]. He showed that there exists an $\alpha > 0$ sufficiently small so that f_γ is not quasiconvex for all $\gamma > 0$, while for every choice of $\alpha > 0$ f_γ is rank one convex for γ small enough. Again f_γ is smooth.

All of these examples share a similar pattern with respect to their convexity properties. More precisely,

1. for each example the function f_γ is convex when $\gamma = 0$,
2. for each example there exist convexity, polyconvexity, quasiconvexity, and rank one convexity thresholds $\gamma_c, \gamma_p, \gamma_q, \gamma_r$ respectively, with the property that for $\gamma \in [0,\infty)$ the function f_γ is

$$\text{convex} \Leftrightarrow \gamma \leq \gamma_c , \tag{3}$$

$$\text{polyconvex} \Leftrightarrow \gamma \leq \gamma_p , \tag{4}$$

$$\text{quasiconvex} \Leftrightarrow \gamma \leq \gamma_q , \tag{5}$$

$$\text{rank one convex} \Leftrightarrow \gamma \leq \gamma_r . \tag{6}$$

3. SOME NUMERICALLY USEFUL CHARACTERIZATIONS OF THE DIFFERENT NOTIONS OF CONVEXITY

We show how the problem of determining whether a function is convex, polyconvex, quasiconvex, or rank one convex reduces to solving an optimization problem. This can be done in several ways depending on the smoothness properties of the function.

Let $f : \mathbb{R}^{m \times n} \to \mathbb{R}$, and suppose that $f \in C^1(\mathbb{R}^{m \times n})$. Let

$$h : \mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n} \to \mathbb{R}$$

be defined as

$$h(\xi, \eta) = f(\xi + \eta) - f(\xi) - \langle \nabla f(\xi) ; \eta \rangle, \quad \xi, \eta \in \mathbb{R}^{m \times n} , \tag{7}$$

and let the function $g : \mathbb{R}^{m \times n} \times \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ be given by

$$g(\xi, a, b) = h(\xi, a \otimes b), \quad \xi \in \mathbb{R}^{m \times n}, a \in \mathbb{R}^m, b \in \mathbb{R}^n . \tag{8}$$

We have the following well-known result (see [12]).

PROPOSITION 3.1: *The function f is convex if and only if*

$$\min_{\xi, \eta} h(\xi, \eta) = 0 . \tag{9}$$

It is rank one convex if and only if

$$\min_{\xi, a, b} g(\xi, a, b) = 0 . \tag{10}$$

If we make no smoothness assumptions on f then checking the convexity of f reduces to solving a constrained optimization problem. More precisely, f is convex if and only if

$$\min_{\xi, \eta, 0 \leq \lambda \leq 1} \{\lambda f(\xi) + (1 - \lambda) f(\eta) - f(\lambda \xi + (1 - \lambda) \eta)\} = 0$$

A similar result holds for rank one convexity provided we take η to be of the form $\xi + a \otimes b$.

There is no practical advantage in using these characterizations, however, since solving a constrained optimization problem, even with only simple bound constraints as is the case here, is harder than solving an unconstrained one.

If we assume that $f \in C^2(\mathbb{R}^{m \times n})$, then it is well known that f is convex if and only if its Hessian $\nabla^2 f(\xi)$ is positive semidefinite for all ξ. If we denote the smallest eigenvalue of the Hessian of f at ξ by $\lambda_{\min}(\xi)$, then we have

$$f \text{ is convex} \Leftrightarrow \inf_{\xi} \lambda_{\min}(\xi) \geq 0 . \tag{11}$$

While there exist efficient algorithms to minimize the smallest eigenvalue of a symmetric matrix depending on a vector of parameters ξ (see Overton [25, 26]), there is again no practical advantage in using the characterization (11) of convexity as eigenvalue minimization is a substantially more difficult problem to solve than (9).

The rank one convexity of f is equivalent to the so called Legendre-Hadamard condition, namely

$$\langle \nabla^2 f(\xi)\, a \otimes b \,;\, a \otimes b \rangle = \sum_{i,j=1}^{m} \sum_{\alpha,\beta=1}^{n} \frac{\partial^2 f(\xi)}{\partial \xi_{i\alpha}\, \partial \xi_{j\beta}} a_i a_j b_\alpha b_\beta \geq 0$$

for all $\xi \in \mathbb{R}^{m \times n}$, $a \in \mathbb{R}^m$ and $b \in \mathbb{R}^n$. Thus

$$f \text{ is rank one convex} \Leftrightarrow \inf_{\xi, a, b} \langle \nabla^2 f(\xi)\, a \otimes b \,;\, a \otimes b \rangle = 0 . \tag{12}$$

Again, this characterization of rank one convexity presents no advantage over (10) from the computational point of view.

When $m = n = 2$, we have the following characterization of the polyconvexity of f (see [12]). For $\xi_i \in \mathbb{R}^{2 \times 2}$, $\lambda_i \in \mathbb{R}$, $1 \leq i \leq 6$ define the function

$$l(\xi_1, \ldots, \xi_6, \lambda_1, \ldots, \lambda_6) = \sum_{i=1}^{6} \lambda_i f(\xi_i) - f\left(\sum_{i=1}^{6} \lambda_i \xi_i\right) \tag{13}$$

and consider the constrained optimization problem

$$\min_{\xi_i, \lambda_i} l(\xi_1, \ldots, \xi_6, \lambda_1, \ldots, \lambda_6) \tag{14}$$

$$\text{s.t.} \quad \lambda_i \geq 0 ,$$

$$\sum_{6} \lambda_i = 1 ,$$

$$\sum_{i=1} \lambda_i \det \xi_i = \det\left(\sum_{i=1}^{6} \lambda_i \xi_i\right) .$$

PROPOSITION 3.2: *f is polyconvex if and only if the optimal value of problem (14) is 0.*

Let us now assume that $f \in C^1(\mathbb{R}^{2 \times 2})$ and for $\xi, \eta, \rho \in \mathbb{R}^{2 \times 2}$ with $\det \eta \neq 0$, $\det \rho \neq 0$, define

$$\tilde{l}(\xi, \eta, \rho) = \frac{f(\xi + \eta) - f(\xi) - \langle \nabla f(\xi) \,;\, \eta \rangle}{\det \eta} - \frac{f(\xi + \rho) - f(\xi) - \langle \nabla f(\xi) \,;\, \rho \rangle}{\det \rho} . \tag{15}$$

Consider the following constrained optimization problem.

$$\inf_{\xi, \eta, \rho} \tilde{I}(\xi, \eta, \rho) \tag{16}$$

$$\text{s.t.} \quad \eta \in \mathbb{R}_+^{2 \times 2}, \text{ i.e. } \det \eta > 0 \, ,$$

$$\rho \in \mathbb{R}_-^{2 \times 2}, \text{ i.e. } \det \rho > 0 \, .$$

We then have the following characterization of polyconvexity (see Aubert [3]).

PROPOSITION, 3.3: *f is polyconvex if and only if the optimal value of problem (16) is 0.*

We now turn to the quasiconvexity case. It is clear from the definition that $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ is quasiconvex if and only if

$$\mathcal{I}(f) \equiv \inf_{\xi \in \mathbb{R}^{m \times n}, \varphi \in W^{1, \infty}(\Omega, \mathbb{R}^m)} \left\{ \int_\Omega [f(\xi + \nabla\varphi(x)) - f(\xi)] \, dx \right\} = 0 \tag{17}$$

for every bounded open subset Ω of $\mathbb{R}^n$. Recall that the infimum in (17) is independent of the choice of Ω (see [12]). Thus, from now on, we take Ω to be a fixed and particularly simple domain, e.g., when $n = 2$, the interior of the unit square $[0, 1] \times [0, 1]$. Let $\mathcal{T}_h$ denote a regular triangulation of Ω of mesh size $h > 0$, and, for a triangle $K \in \mathcal{T}_h$, let $\mathcal{P}_1(K)$ denote the space of polynomial functions of degree one on K. Consider the finite dimensional subspace U_h of $W_0^{1,\infty}(\Omega, \mathbb{R}^m)$ defined by

$$U_h = \underbrace{V_h \times \cdots \times V_h}_{m}$$

where

$$V_h = \{ u : \Omega \to \mathbb{R} \text{ continuous} : u|_K \in \mathcal{P}_1(K) \text{ for every } K \in \mathcal{T}_h \text{ and } u|_{\partial\Omega} = 0 \} \, .$$

Let n_h denote the dimension of V_h. The function

$$(\xi, \varphi) \mapsto \int_\Omega [f(\xi + \nabla\varphi(x)) - f(\xi)] \, dx$$

becomes a function

$$k = k_h : \mathbb{R}^{m \times n} \times \mathbb{R}^{mn_h} \to \mathbb{R} \, . \tag{18}$$

Consider

$$\mathcal{I}_h(f) \equiv \inf_{\xi \in \mathbb{R}^{m \times n}, \varphi \in U_h} k(\xi, \varphi) \, . \tag{19}$$

One can show that (see [6])

$$\mathcal{I}(f) = \lim_{h \to 0} \mathcal{I}_h(f) \, . \tag{20}$$

Since it is obvious from the definition (19) that $\mathcal{I}_h(f) \leq 0$ for every $h > 0$, the following result follows from (20).

PROPOSITION 3.4: *The function f is quasiconvex if and only if $\mathcal{I}_h(f) = 0$ for every $h > 0$.*

It is possible to replace the space V_h by the space $\tilde{V}_h$ of continuous functions $u : \Omega \to \mathbb{R}$ that satisfy $u|_K \in \mathscr{P}_1(K)$ but are periodic on the boundary $\partial\Omega$ (see [30] for example), and to use the space

$$\tilde{U}_h = \underbrace{\tilde{V}_h \times \cdots \times \tilde{V}_h}_{h \quad m}$$

in place of U_h. Proposition (3.4) still holds.

In our numerical investigations we have used the characterizations of convexity, rank one convexity, polyconvexity, and quasiconvexity provided by propositions (3.1), (3.2), (3.3) and (3.4).

4. ALGORITHMS

We describe two numerical schemes for checking the convexity, polyconvexity, quasiconvexity, and rank one convexity of a function such as those introduced in Section 2. More precisely, we wish to determine numerically the values of the thresholds γ_c, γ_p,γ_q, γ_r defined in (3), (4), (5), (6) respectively.

The first scheme, which we shall call the direct method, has the advantage of simplicity and reliability, but is somehow inefficient. The second one, which we shall call the pq-method, is several order of magnitudes faster than the direct method, but will occasionally fail to compute the correct value of the threshold.

We consider a function $f_\gamma : \mathbb{R}^{m \times n} \to \mathbb{R}$ that is affine in γ, namely

$$f_\gamma(\xi) = f_1(\xi) + \gamma f_2(\xi)$$

with $f_1, f_2 \in C^1(\mathbb{R}^{m \times n})$ and f_1 convex. Observe that all of the functions described in Section 2 are of this form for suitable values of m and n. Recall the function $h_\gamma : \mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n} \to \mathbb{R}$ defined in (7), namely

$$h_\gamma(\xi, \eta) = f_\gamma(\xi + \eta) - f_\gamma(\xi) - \langle \nabla f_\gamma(\xi) ; \eta \rangle .$$

It can be written as

$$h_\gamma(\xi, \eta) = p(\xi, \eta) + \gamma q(\xi, \eta)$$

where

$$p(\xi, \eta) = f_1(\xi + \eta) - f_1(\xi) - \langle \nabla f_1(\xi) ; \eta \rangle$$

$$q(\xi, \eta) = f_2(\xi + \eta) - f_2(\xi) - \langle \nabla f_2(\xi) ; \eta \rangle .$$

Since f_1 is convex by assumption, $p(\xi, \eta) \geqslant 0$ for all $\xi, \eta \in \mathbb{R}^{m \times n}$. Similarly, the functions g_γ, l_γ, $\tilde{l}_\gamma$ and k_γ defined in (8), (13), (15) and (18) respectively, are all of the form

$$p + \gamma q$$

for suitable functions p and q with $p \geqslant 0$. Thus, from an algorithmic point of view, determining the convexity, polyconvexity, quasiconvexity, and rank one convexity thresholds are all particular instances of the very same problem, namely, given a function

$$\phi_\gamma(x) = p(x) + \gamma q(x), \quad x \in \mathbb{R}^k \tag{21}$$

with $p(x) \geqslant 0$ for all $x \in \mathbb{R}^k$, determine the value γ^+ of the parameter γ with the property that for $\gamma \geqslant 0$

$$\phi_\gamma(x) \geqslant 0 \text{ for all } x \in \mathbb{R}^k \Leftrightarrow \gamma \in [0, \gamma^+] .$$

Observe that γ^+ is well defined provided ϕ_γ takes on negative values for γ large enough Thus we make the following assumptions on ϕ_γ

1 $p(x) \geqslant 0$ for all $x \in \mathbb{R}^k$,

2 $q(x) < 0$ for some $x \in \mathbb{R}^k$

Now we describe the *direct method* to compute γ^+

ALGORITHM 4 1 *The direct method*

1 *Choose an initial value of* γ *large enough that* $\phi_\gamma(x) < 0$ *for some* $x \in \mathbb{R}^k$

2 *Use a minimization algorithm to compute a point* x *for which* $\phi_\gamma(x) < 0$

3 *Set* γ *equal to* $-\dfrac{p(x)}{q(x)}$

4 *Go to step 2*

The algorithm terminates when the optimization process in step 2 fails to determine an x with $\phi_\gamma(x) < 0$ The current value of γ is then the computed approximation of γ^+ Step 3 is justified as follows Given a value of γ and a point x_γ with $\phi_\gamma(x_\gamma) < 0$, let

$$\bar{\gamma} = -\frac{p(x_\gamma)}{q(x_\gamma)}$$

Then $\phi_\gamma(x_\gamma) < 0$ for every $\gamma > \bar{\gamma}$ Hence, $\gamma^+ \leqslant \bar{\gamma}$

Of course, the performance of this scheme is completely dependent on the choice of the optimization algorithm in step 2 We will address this issue in the next section It is clear, however, that this method is inherently inefficient, since we can expect to have to solve a great many optimization problems before a good approximation to γ^+ is obtained

Remark 4 1 Suppose that the functions p and q are homogeneous of degree $\nu > 0$ Then so is ϕ_γ and we have

$$\inf_{x \in \mathbb{R}^k} \phi_\gamma(x) = \begin{cases} 0 & \text{if } 0 \leqslant \gamma \leqslant \gamma^+ \\ -\infty & \text{if } \gamma > \gamma^+ \end{cases}$$

Note that this is the case when studying the convexity, quasiconvexity, or rank one convexity of the functions f_γ in examples 1, 2 and 3 Indeed, the functions h_γ, g_γ and k_γ are homogeneous of the same degree as f_γ

Now we describe the second scheme for computing γ^+ In general, for a function ϕ_γ as in (21), there exist values $\gamma^- \leqslant 0 \leqslant \gamma^+$ such that

$$\phi_\gamma(x) \geqslant 0 \text{ for all } x \in \mathbb{R}^k \Leftrightarrow \gamma \in [\gamma\ , \gamma^+]$$

Again we assume that ϕ_γ takes on negative values for sufficiently large negative γ Now, since $p(x) \geqslant 0$ for all $x \in \mathbb{R}^k$, we have

$$\phi_\gamma(x) \geqslant 0 \text{ for all } x \Leftrightarrow p(x) \geqslant -\gamma q(x) \text{ for all } x$$

$$\Leftrightarrow \begin{cases} -\dfrac{p(x)}{q(x)} \geqslant \gamma \text{ for all } x \text{ with } q(x) < 0 \\ -\dfrac{p(x)}{q(x)} \leqslant \gamma \text{ for all } x \text{ with } q(x) > 0 \end{cases}$$

$$\Leftrightarrow \gamma^- \equiv \sup_{q(x) > 0} -\frac{p(x)}{q(x)} \leqslant \gamma \leqslant \gamma^+ \equiv \inf_{q(x) < 0} -\frac{p(x)}{q(x)}$$

Hence

$$\min\{\gamma^+, -\gamma^-\} = \inf_x \frac{p(x)}{|q(x)|}.$$

so that if $\gamma^+ \leqslant -\gamma^-$, then

$$\gamma^+ = \inf_x \frac{p(x)}{|q(x)|}. \tag{22}$$

Thus we have the following pair of algorithms.

ALGORITHM 4.2: *The pq-method: unconstrained case. Suppose that* $\gamma^+ \leqslant |\gamma^-|$. *Then* γ^+ *is computed as the optimal value of the following optimization problem:*

$$\inf\left\{\frac{p(x)}{|q(x)|} : x \in \mathbb{R}^k\right\}$$

ALGORITHM 4.3: *The pq-method: constrained case. Suppose that* $\gamma^+ > |\gamma^-|$. *Then* γ^+ *is computed as the optimal value of the following constrained optimization problem:*

$$\inf\left\{-\frac{p(x)}{q(x)} : x \in \mathbb{R}^k \text{ with } q(x) < 0\right\}$$

5. THE OPTIMIZATION ALGORITHMS

We now turn to a discussion of the methods that are used to solve the optimization problems in algorithms (4.1), (4.2) and (4.3). An extensive discussion of optimization techniques can be found in e.g. [17, 24], while [22] provides a guide to available software, both commercial and public domain.

Two of the most widely used unconstrained optimization techniques are the conjugate gradient methods and the variable metric methods. Conjugate gradient methods, of which the Polak-Ribière method, or modifications of it, is usually thought to be the most effective, are particularly well suited for large scale problems due to their low storage requirements. Variable metric methods, of which the BFGS method is usually thought to be the most efficient, have much higher storage requirements and so are better suited to small and medium scale problems. (Limited memory BFGS methods [21] alleviate this problem, but we did not use these techniques.) We used the routine CONMIN of Shanno and Phua [29]. CONMIN implements both the BFGS method and a modification of the Polak-Ribière conjugate gradient method due to Shanno [28], with the choice of the method left to the user. Both algorithms use a cubic interpolation for the line search. This routine, written in FORTRAN, is algorithm 500 of TOMS and is available on Netlib.

Of course, none of these methods is guaranteed to converge to a global minimum of the function. Since the optimization problems to be solved are global optimization problems, we have also considered some stochastic algorithms designed to avoid being trapped at a local minimum. First we considered a simulated annealing version of the classical Nelder-Meade simplex method given in [27]. This method only requires function evaluations and makes no use of gradient information. However, it is only suitable for small scale problems due to high storage requirements. We also considered a method based on stochastic differential equations [2, 18]. This is essentially the gradient method perturbed by a stochastic term that vanishes asymptotically, thus compounding the inefficiency of the gradient method with the inefficiency inherent to a stochastic method. It has been proved, however, that, under suitable assumptions on the function to minimize, the method converges towards the global minimum in some probabilistic sense. Furthermore, the method has very low storage requirements, and is therefore suited for large scale problems. Gremaud [18] used also a modified version of the algorithm, replacing the gradient method by the Polak-Ribière conjugate gradient method, thereby improving on the efficiency. No proof of convergence to a global minimum exists for the modified version, however. Another possible approach which we have not explored is to make use of evolutionary algorithms, especially evolutionary strategies (see Tomassini [31] for a survey of the methods and a guide to further literature). These methods appear to be better suited to small scale problems, however.

To solve the constrained optimization problems, we used the routine FSQP of Zhou and Tits [32]. FSQP is based on sequential quadratic programming. It is very versatile, and can handle simple bounds as well as linear and nonlinear equality and inequality constraints. The routine is written in FORTRAN and is available from the authors.

6. NUMERICAL RESULTS

In this section we present the results of our numerical investigations on the families of functions introduced in Section 2. We compare our results with the small number of known theoretical values and with the few values computed in [13, 18].

We compute the values of γ_c, γ_q and γ_r for hundreds of values of α in examples 1 and 2. We invest considerably less effort in the computation of the polyconvexity threshold γ_p. Indeed, we only estimate γ_p for the family of functions of example 1 and for about 20 different values of α. This is only due to the fact that computing γ_p is of considerably less theoretical interest than estimating γ_q and γ_r, and not a reflection of the relative merits of the algorithms.

In the examples of Section 2 we have $n = 2$ and, for the computations of γ_q, Ω is taken to be the interior of the unit square $[0, 1] \times [0, 1]$. The triangulations $\mathcal{T}_h$ are constructed as follows. We choose an integer s and we partition the interval $[0, 1]$ into s subintervals of equal length, and then divide each resulting square into two triangles, for a total of $2s^2$ triangles. So the mesh size h is equal to $1/s$, and the dimension of the space U_h, corresponding to zero boundary conditions, is equal to $m(s-1)^2$, while that of $\tilde{U}_h$, corresponding to periodic boundary conditions, is $m[(s-1)^2 + 2(s-1) + 1] = ms^2$. We consider values of s ranging from 20 to 100. In the case of zero boundary conditions, the number of variables of the optimization problems then ranges from 726 to 19606 for $m = 2$, and from 1089 to 29409 for $m = 3$. With periodic boundary conditions, these ranges become 804 to 20004 for $m = 2$, and 1206 to 30006 for $m = 3$.

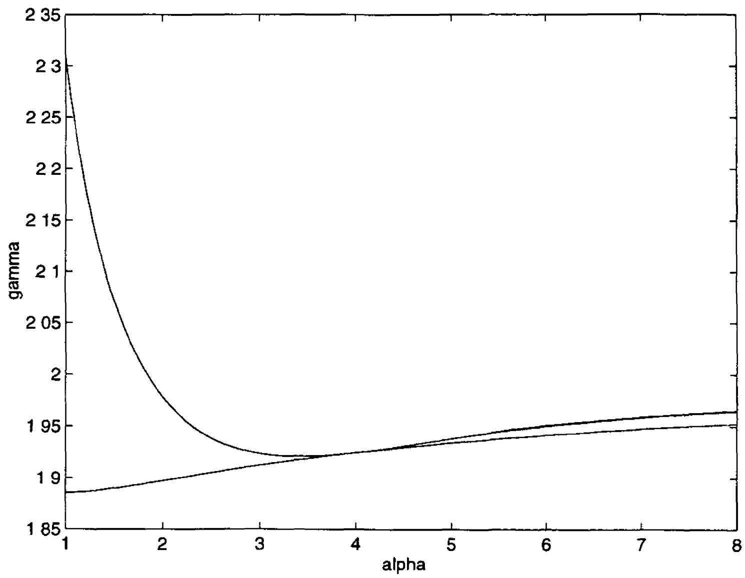


Figure 1. — Graphs of γ vs α for convexity, quasiconvexity, and rank one convexity for example 1. The bottom curve is γ_c, the next highest is γ_r, and the top one is γ_q (note that the curves for rank one convexity and quasiconvexity are, here, indistinguishable).

All the coding was done in FORTRAN and C++ and made use of the BLAS level one. All computations were run on Silicon Graphics workstations equipped with R4000, R4400 and R8000 processors.

6.1. Example 1

We compute γ_c, γ_r, γ_q, for α between 1 and 8 in steps of 0.01. The results are displayed in figure 1, where the values of γ_c, γ_r and γ_q are plotted as functions of α. The γ_c and γ_q curves are computed using the function h of (7) and k of (18) respectively, and the pq-method together with the minimization algorithm of Shanno and Phua. The mesh size h is 1/20 and we used periodic boundary conditions. The minimization algorithm is initialized with a random starting point for $\alpha = 1$. Henceforth, the starting point is taken to be the computed solution at the previous value of α. The γ_r curve is computed using the function g of (8) and the simulated annealing version of the Nelder-Meade algorithm. The minimization routine is initialized with a random starting point for every value of α.

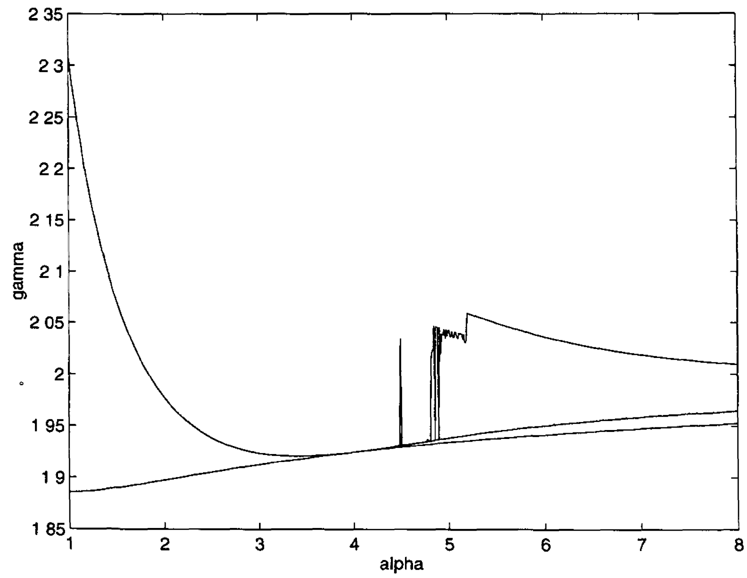


Figure 2. — Graphs of γ vs α for convexity, quasiconvexity, and randk one convexity for example 1 with random starting point. The bottom curve is γ_c, the next highest γ_r, and the top one γ_q

We see that the γ_r and γ_q curves are nearly indistinguishable. Indeed, the largest gap between the computed values of γ_r and γ_q was about 9.2×10^{-4}.

When $\alpha = 1$, so that the correct values of γ_c and γ_r are known, the results were as follows:

	computed value	correct value	error
γ_c	1.88561822236594	1.88561808316413	$\sim 1.4 \times 10^{-7}$
γ_r	2.30941239674591	2.3094010767585	$\sim 1.2 \times 10^{-5}$

More generally, the worst error between the computed values of γ_r and the exact values, when known, was about 1.4×10^{-3}.

A few values of γ_q have been estimated before. Dacorogna-Douchet-Gangbo-Rappaz [13] best estimation of γ_q was 2.33 when $\alpha = 1$ and with $h = 1/10$. Gremaud [18] estimated γ_q for $\alpha = 1, 2, 6$. The following table holds his results, obtained with $h = 1/40$, and ours, obtained with $h = 1/20$.

α	Gremaud's results	our results
1	2.31	2.3094
2	1.9788	1.9779
6	1.9506	1.9510

Thus the results are comparable, with ours slightly better. Recall that Gremaud's computations used a stochastic algorithm designed to locate the global minimum of the function, while ours used a deterministic algorithm unable to distinguish between local and global minima. Nonetheless, the stochastic algorithm was unable to find better values than the deterministic one. This is very interesting, since the pq-method may indeed encounter difficulties with local minima. This is illustrated in figure 2. Again the γ_c, γ_r and γ_q curves are plotted as functions of α. But now, the minimization routine for the computation of γ_q is initialized with a random starting point for every value of α. We see that for larger values of α, the algorithm grossly overestimated the value of γ_q.

Finally, in figures 3 and 4, we illustrate the effect of the choice of boundary conditions on the solutions. Figure 3 shows the graph of one component of the solution for the computed γ_q with $\alpha = 1$ that satisfies zero boundary conditions. The graph is displayed from two different points of view to emphasize the oscillatory structure of the function. Figure 3 shows the same component of the solution to the same problem but satisfying periodic boundary conditions. In both cases the mesh size is $h = 1/100$.

We now discuss our estimates of the polyconvexity threshold γ_p. We computed γ_p only for a few values of α. The results are presented in the following table, where we compare our estimated γ_p and γ_r. The values of γ_p are obtained by applying the pq-method to the function given in Proposition (3.3). The resulting constrained optimization problem is solved by calling the FSQP routine of Zhou and Tits [32].

The most interesting characteristics of our results are as follows. For $\alpha \in [1, 1.83]$, so that $\gamma_r \geqslant 2.0$, our estimated γ_p is precisely equal to 2.0. For $\alpha \geqslant 1.84$, so that $\gamma_r < 2.0$, our estimated γ_p and γ_r are nearly equal. When the correct value of γ_r is known, it agrees with our computed γ_p for the first seven or eight digits. Observe that $\gamma = 2$ is the positivity constant of the family of functions f_γ, namely

$$f_\gamma(\xi) \geqslant 0 \text{ for every } \xi \in \mathbb{R}^{2\times 2} \Leftrightarrow \gamma \geqslant 2$$

independently of α.

α	γ_p	γ_r	correct value of γ_r
1.0	2.00000000000	2.30941239675	2.30940107675
1.3	2.00000000000	2.13978159870	
1.5	2.00000000000	2.07165338144	
1.7	2.00000000000	2.02426844298	
1.83	2.00000000000	2.00123065553	
1.84	1.99964675082	1.99965701190	
1.85	1.9981030331	1.99811528459	
2.0	1.97785385481	1.97786450188	
2.4	1.94366150361	1.94369216373	
2.5	1.93831887377	1.93832149662	
3.0	1.92351225803	1.92354680800	
3.4	1.92083353227	1.92083418964	
4.0	1.92450104807	1.92452092029	
4.3	1.92811055074	1.92812897070	
5.0	1.93808947291	1.93813153935	
5.5	1.94475510544	1.94496424134	1.94475498595
6.0	1.95014629012	1.95025051423	1.95014618758
6.5	1.95459027804	1.95467088467	1.95459028046
7.0	1.95831495997	1.95845384478	1.95831484750
7.5	1.96148033948	1.96282698317	1.96148034012
8.0	1.96420320692	1.96474159128	1.96420303878

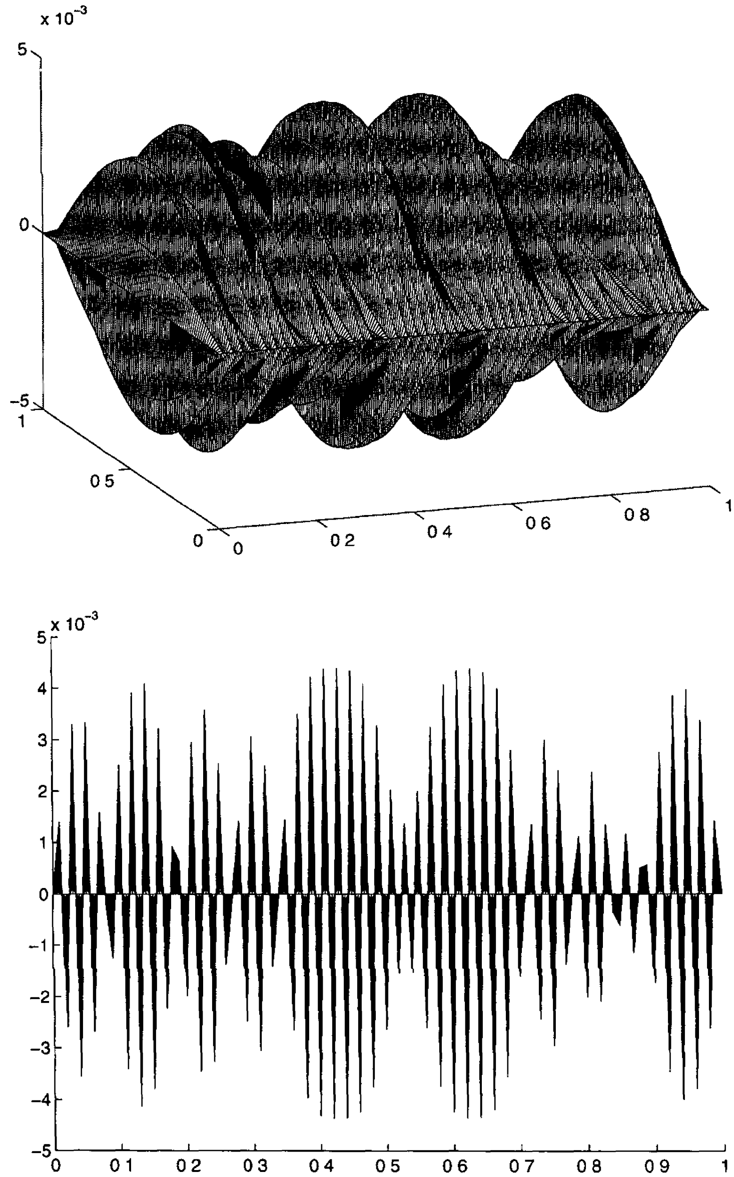


Figure 3. — Graph of one component of the solution with 0 boundary conditions for quasiconvexity in example 1 with $\alpha = 1$, viewed from two different angles. The bottom figure illustrates clearly the oscillatory structure of the function.

6.2. Example 2

We compute the values of γ_c, γ_r and γ_q for α between 1 and 3 in steps of 0.01. The results are displayed in figure 5. The γ_c and γ_r curves are computed with the simulated annealing version of the Nelder-Meade algorithm. The minimization routine is initialized with a random starting point for every value of α. The γ_q curve is computed via the pq-method and the minimization algorithm of Shanno and Phua. The minimization algorithm is initialized with a random starting point for $\alpha = 1$. Henceforth, the starting point is taken to be the computed solution at

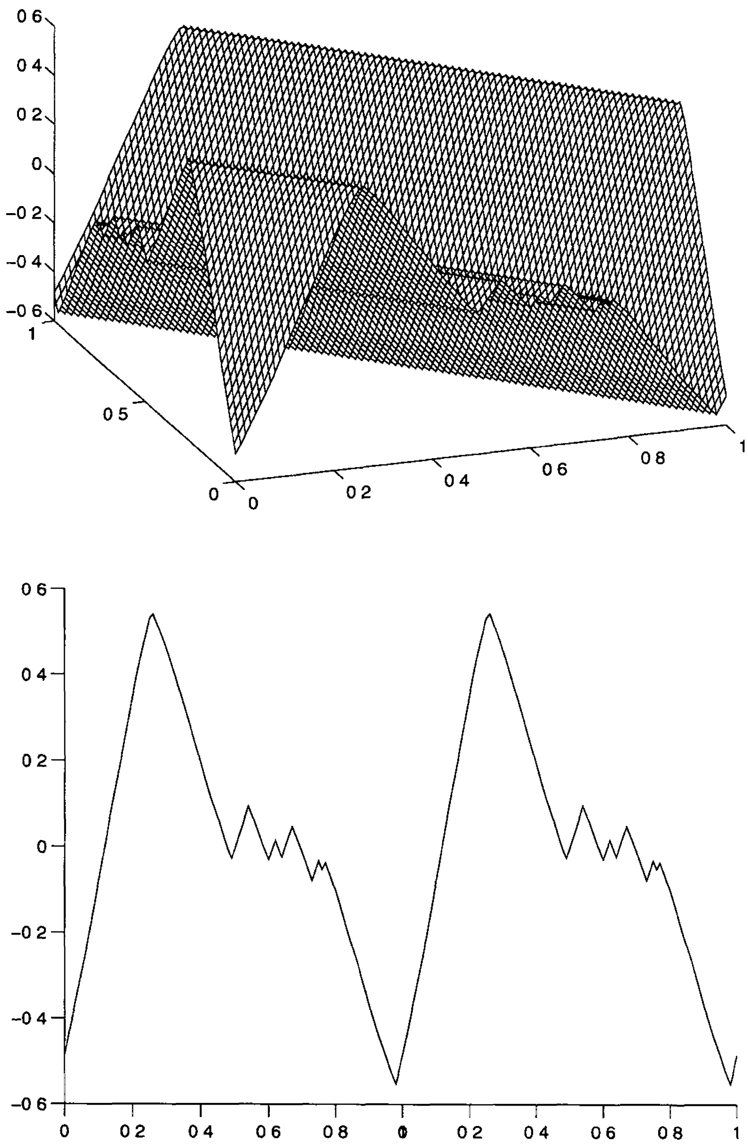
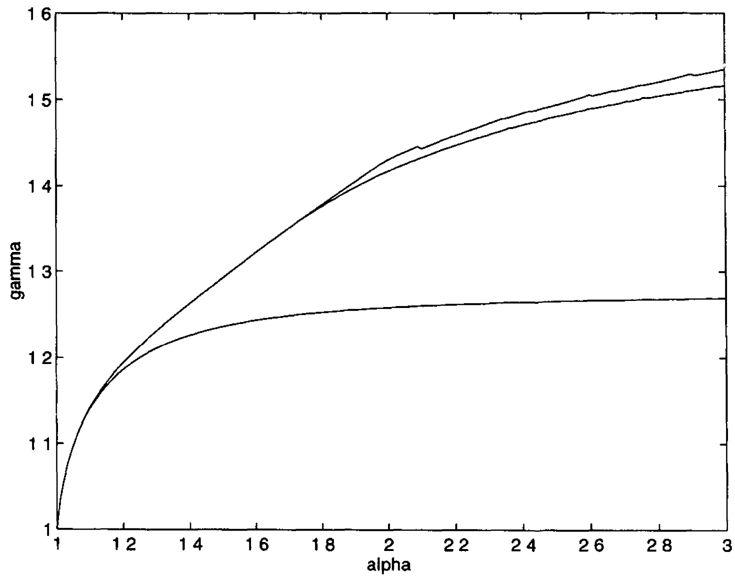


Figure 4. — Graph of one component of the solution with periodic boundary conditions for quasiconvexity in example 1 with $\alpha = 1$, viewed from two different angles. The bottom figure illustrates clearly the oscillatory structure of the function.

the previous value of α. In figure 5 the mesh size h is 1/20 for the first graph, and we observe convergence problems in the computation of γ_q for larger values of α. In the second graph of figure 5, the mesh size is increased to 1/50, and the γ_r and γ_q curves then become indistinguishable.

The worst error between the computed value of γ_r and the correct values was about 1.8×10^{-3}, while the largest gap between the computed values of γ_r and γ_q, with $h = 1/50$, was about 1.4×10^{-3}. When $\alpha = 1$, the computed value of γ_q was 1.00000808500197, yielding an error of order 10^{-6}. The gap between the computed γ_r and γ_q increases as α approaches 3.



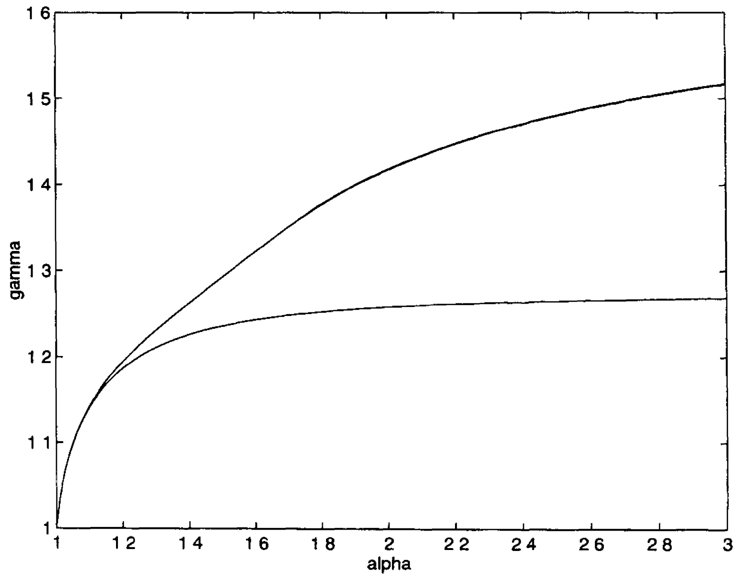


Figure 5. — Graphs of γ vs α for convexity, quasiconvexity, and rank one convexity for example 2 with a 20×20 grid (top graph) and a 50×50 grid (bottom graph). The bottom curve is γ_c, the next highest is γ_r, and the top one is γ_q.

Gremaud [18] estimated γ_q for $\alpha = 1.5$ and $\alpha = 2$. His computations were done with $h = 1/20$. We compare his results and ours in the following table.

α	Gremaud's results	our results (h = 1/20)	our results (h = 1/50)
1.5	1.2946	1.2927	1.2927
2	1.4237	1.4306	1.4179

Again the results are comparable, with ours slightly better demonstrating again that the stochastic method unable to produce better results than the deterministic ones. Overall, example 2 appears slightly less amenable to numerical investigation than example 1. Local minima cause difficulties for the computation of γ_q for all values of α in the chosen interval [1, 3].

6.3. Example 3

We compute the values of γ_r and γ_q for several choices of eigenvalues of the matrix M. We use the simulated annealing version of the Nelder-Meade algorithm to compute γ_r and the direct method together with the minimization algorithm of Shanno and Phua for γ_q. The mesh size is 1/20. (Observe that here, $|\gamma_q^-| \neq \gamma_q^+$ in general). The results are summarized in the table below.

Again, we see that the computed value of γ_q is larger than γ_r in all fifteen examples we considered, while the difference between these quantities is at most 6×10^{-4}, often much less.

Eigenvalues	γ_r	computed value of γ_r	computed value of γ_q
(2, 1, 1, 0)	2/3	0.66666846	0.66678419
(2, 1, 1, 1/2	2	2.0000070	2.0001304
(3, 2, 2, 1)	2	2.0000092	2.0004091
(4, 2, 2, 1)	1	1.0000063	1.0001142
(6, 2, 2, 1)	1/3	0.33486164	0.33334408
(8, 2, 2, 1)	1/5	0.20084300	0.20000793
(5, 4, 4, 2)	2	2.0000268	2.0005941
(− 1, − 2, − 2, − 3)	2/9	0.22222251	0.22223656
(− 1, − 3, − 3, − 4)	1/6	0.16666681	0.16667002
(− 2, − 3, − 3, − 4)	2/11	0.18181862	0.18182958
(− 1, − 4, − 4, − 5)	1/8	0.12508059	0.12500245
(− 1, − 2, − 2, − 4)	2/13	0.15384647	0.15387374
(− 1, − 7/2, − 7/2, − 5)	4/31	0.12903249	0.12905427
(3, 2, 1, 0)	2/5	0.40007437	0.40021655
(8, 2, 1, 0)	1/7	0.14340791	0.14286232

6.4. Example 4

This is the celebrated example of Sverak, providing an example of a function that is rank one convex but not quasiconvex. Here $m = 3$. We chose $\alpha = 1/100$. For this value of α, we know that $\gamma_q = 0$, while $\gamma_r > 0$. We computed γ_r and γ_q with the direct method together with the Shanno-Phua minimization algorithm, and with periodic boundary conditions. We found

$$\gamma_r \approx 0.12978763$$

and

$$\gamma_q \approx \begin{cases} 1.33 \times 10^{-11} & \text{with mesh size } 1/20 \\ 1.08 \times 10^{-11} & \text{with mesh size } 1/100 \end{cases}$$

Thus our algorithms had no difficulties computing the correct value of γ_q in this case. The reader may be interested to compare the graphs of the three components of the computed solution for the estimation of γ_q with the specific example of a quasiconvex function that is not rank one convex given by Sverak [30], namely

$$\varphi(x, y) = (\sin x, \sin y, \sin(x + y)) .$$

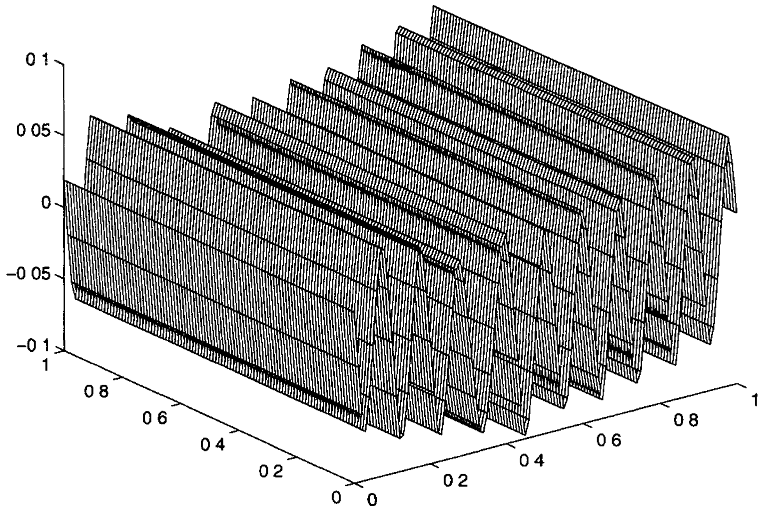


Figure 6. — Graph of the first component of the solution function for the estimation of γ_q in Sverak's example. The mesh size = 1/100.

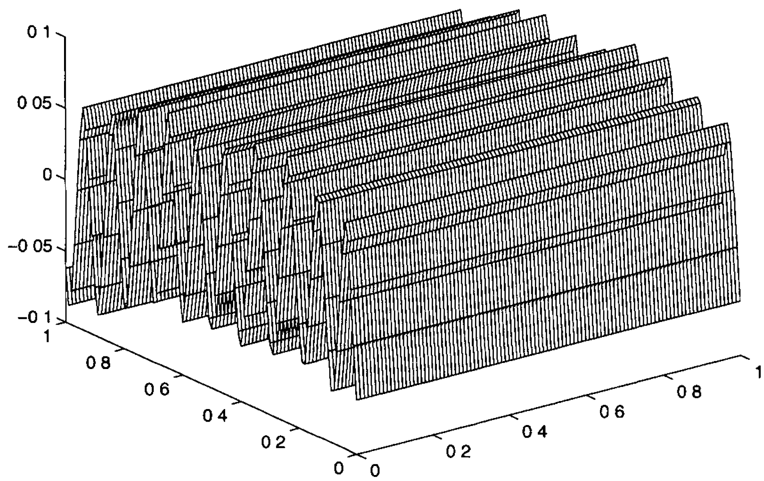


Figure 7. — Graph of the second component of the solution function for the estimation of γ_q in Sverak's example. The mesh size = 1/100.

7. MORE NUMERICAL RESULTS

We considered several other families of functions in addition to those introduced in Section 2, both in the case $m = 2$ and $m = 3$. All of these functions are of the form

$$f_\gamma(\xi) = f_1(\xi) + \gamma f_2(\xi)$$

with f_1 convex. No analytical results are known concerning the values of γ_c, γ_p, γ_q or γ_r. In all of these examples, we found our estimations of γ_q and γ_r to be essentially equal.

In dimension 2, we have considered the following families of functions.

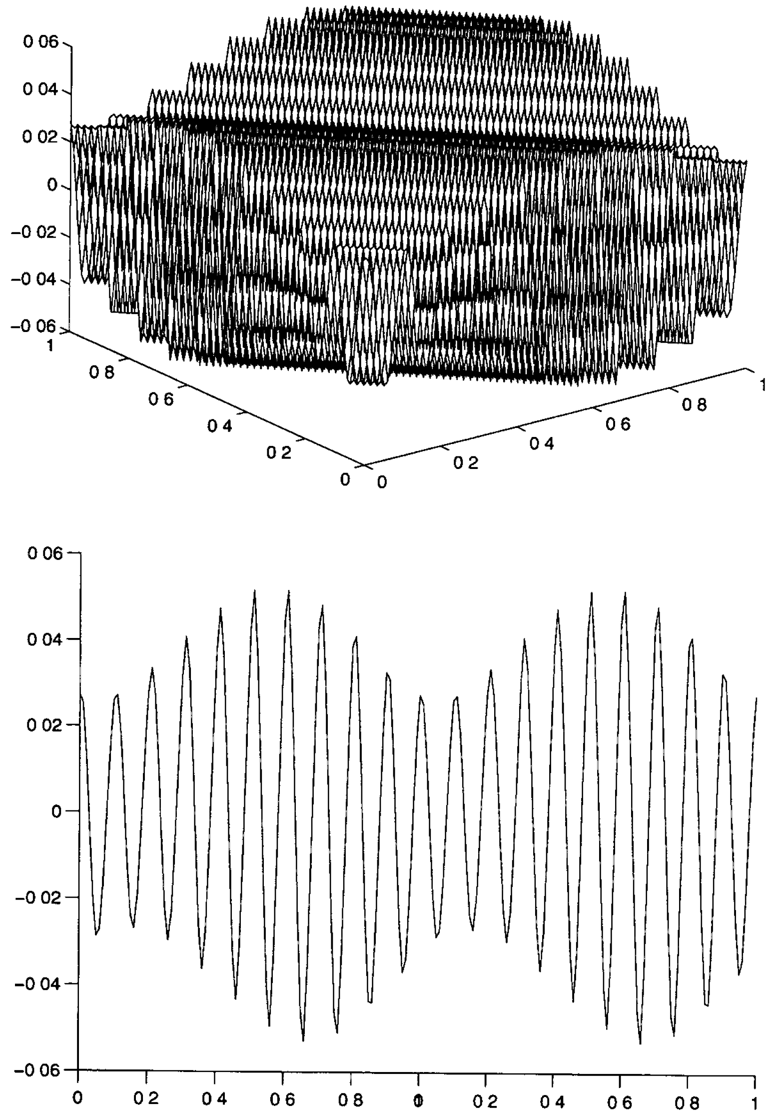


Figure 8. — Graph of the third component of the solution function for the estimation of γ_q in Sverak's example, viewed from two different angles. The bottom figure illustrates clearly the oscillatory structure of the function. The mesh size = 1/100.

1.

$$f_\gamma(\xi) = \begin{cases} |\xi| + \gamma \dfrac{\langle M\xi\,;\,\xi\rangle}{|\xi|} & \text{if } \xi \neq 0 \\ 0 & \text{if } \xi = 0 \end{cases}$$

that is f_γ is the function of example 3 except that now M is an arbitrary 4×4 symmetric matrix. We tried many different choices for M.

2.

$$f_\gamma(\xi) = |\xi|^4 + |\xi|^2 + \gamma a(\xi)$$

where $a(\xi)$ is a polynomial of degree 3 in the four entries of ξ. There are 20 monomials of this type, and the function $a(\xi)$ is completely determined by the corresponding coefficients. We tried many different possible choices of coefficients.

In dimension 3 we considered the following functions.

1.

$$f_\gamma(\xi) = |\xi|^{2\alpha}(|\xi|^2 - \gamma\rho(\xi))$$

with the following choices of functions $\rho(\xi)$,

$$\rho(\xi) = \begin{cases} |\mathrm{adj}\,(\xi)| \\ \xi_{11}\,\xi_{22} - \xi_{12}\,\xi_{21} \\ \xi_{11}\,\xi_{22} - \xi_{12}\,\xi_{21} + \xi_{11}\,\xi_{32} - \xi_{12}\,\xi_{31} \\ \xi_{11}\,\xi_{22} - \xi_{12}\,\xi_{21} + \xi_{11}\,\xi_{32} - \xi_{12}\,\xi_{31} + \xi_{21}\,\xi_{32} - \xi_{22}\,\xi_{31} \end{cases}$$

2.

$$f_\gamma(\xi) = |\xi|^4 - \gamma|\mathrm{adj}\,(\xi)|^2$$

3.

$$f_\gamma(\xi) = |\xi|^8 - \gamma|\mathrm{adj}\,(\xi)|^4$$

4.

$$f_\gamma(\xi) = |\xi|^8 - \gamma(|\xi|^2(\xi_{11}\,\xi_{22} - \xi_{12}\,\xi_{21}) + (\xi_{11}\,\xi_{32} - \xi_{12}\,\xi_{31})^2 + (\xi_{21}\,\xi_{32} - \xi_{22}\,\xi_{31})^2)$$

8. SUMMARY AND CONCLUSIONS

We summarize the most important features of our numerical results.

- Our computations are in excellent agreement with all the known analytical results. In particular, we had no trouble recovering Sverak's example of a function that is rank one convex but not quasiconvex.
- The stochastic methods failed to produce better results than the deterministic methods.
- The use of periodic boundary conditions provides slightly better estimates of γ_q than those obtained with zero boundary conditions.
- Refining the mesh does not yield significantly better results for the estimation of γ_q.
- In every example considered in dimension 2, the estimated values of γ_q and γ_r are nearly equal.

It is currently not known whether a function

$$f : \mathbb{R}^{2\times 2} \to \mathbb{R}$$

is quasiconvex if and only if it is rank one convex. Our numerical experiments provide some evidence that, for the examples considered, this is indeed the case.

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