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Regularity of Minimizers in Nonlinear Elasticity – the Case of a One-Well Problem in Nonlinear Elasticity

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In this note sufficient conditions for bounds on the deformation gradient of a minimizer of a variational problem in nonlinear elasticity are reviewed. As a specific model class, energy densities which are the relaxation of the squared distance function to compact sets are considered and estimates in the space of functions with bounded oscillation are presented. An explicit example related to a one-well problem shows that assumptions of convexity are essential for uniform bounds on the deformation gradient. As an application of the relaxation of the energy in this special case it is indicated how general relaxation formulas for energies with p-growth can be obtained if the relaxation with quadratic growth satisfies natural assumptions.

1 Introduction

Variational models in nonlinear elasticity play a fundamental role in modern applications in the engineering sciences. It has long been recognized that linear models are inappropriate to capture the true elastic behavior of materials with internal structures which have a significant impact on the response of the materials to applied loads. Significant progress in the mathematical analysis of these models has been achieved, in particular following the seminal paper Ball (1976/77) which identified classes of energy densities for which existence of solutions for the corresponding variational problems can be inferred with the direct method in the calculus of variations.

Despite significant progress in the past years, many questions concerning regularity and uniqueness of solutions remain open. In this note we focus on the question of uniform estimates for the gradient of minimizers. This question has direct applications to the material systems modeled by the variational principles: a minimizer u represents the deformation and its gradient describes local changes of length. It seems a natural requirement that this quantity be bounded in an energy minimizing configuration.

In order to illustrate some of the effects that may occur we recall some recent results on regularity of minimizers in Dolzmann et al. (2011) and confront them with a special model example, the nonlinear version of a one-well energy in two dimensions, which serves as the most basic model for the austenitic phase of a material undergoing an austenite-martensite phase transformation in the solid state, see, e.g., Ball and James (1987, 1992); Chipot and Kinderlehrer (1988) for discussions from the point of view of nonlinear elasticity. We provide a short proof for the well-known relaxation of this energy and indicate a general method that allows one to obtain the relaxation of a corresponding energy with p-growth, $p \geq 2$. These energies fit into the framework of isotropic functions which have been studied in detail in the literature, see, e.g., Šilhavý (2001, 2007b) and the references therein for more general results.

2 Preliminaries

We use standard notation for Lebesgue and Sobolev spaces. The space of all real $m \times n$ matrices is denoted by $\mathbb{M}^{m\times n}$. In 2×2-matrices we use the decomposition into a conformal and anticonformal part, $X = X^+ + X^-$ which is orthogonal with respect to the inner product in $\mathbb{M}^{2\times 2}$ and is given by

$$X^+ = \frac{1}{2}\begin{pmatrix} a & -b \\ b & a \end{pmatrix}, \quad X^- = \frac{1}{2}\begin{pmatrix} c & d \\ d & -c \end{pmatrix}, \tag{1}$$

where $a = X_{11} + X_{22}$, $b = X_{21} - X_{12}$, $c = X_{11} - X_{22}$, and $d = X_{21} + X_{12}$ In particular

$$2 \det X = |X^+|^2 - |X^-|^2 . \tag{2}$$

We finally recall the relevant notions of convexity, see Dacorogna (1989) for more information. Let $f\colon \mathbb{M}^{m\times n} \to \mathbb{R}$ be a real valued function. We say that f is

(a) rank-one convex, if f is convex along rank-one lines, i.e., for all $X \in \mathbb{M}^{m\times n}$ and all $R \in \mathbb{M}^{m\times n}$ with $\mathrm{rank}(R) = 1$ the real-valued function of one variable $t \mapsto f(X + tR)$ is convex; the function is said to be rank-one affine if it is affine along all rank-one lines;

(b) quasiconvex (in the sense of Morrey), if for all $\phi \in C_0^\infty((0,1)^n; \mathbb{R}^m)$ and all $X \in \mathbb{M}^{m\times n}$ in inequality

$$f(X) \leq \int_{(0,1)^n} f\big(X + \nabla\Phi(x)\big)\mathrm{d}x$$

holds; the function is said to be quasiaffine if equality holds in this inequality for all ϕ;

(c) polyconvex, if f can be represented as a convex function g of X and all its minors, i.e., all subdeterminants of X; the function is said to be polyaffine if g is affine.

It is important to note the following implications:

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

In case that a given function f fails to be polyconvex (quasiconvex, rank-one convex) one defines the polyconvex (quasiconvex, rank-one convex) envelope of the function as the largest polyconvex (quasiconvex, rank-one convex) function less than or equal to f. For example, the polyconvex envelope is given by

$$f^{\mathrm{pc}}(X) = \sup\big\{p(X)\colon p \text{ is polyconvex with } p \leq f \text{ on } \mathbb{M}^{m\times n}\big\} .$$

In particular, the implications between the notions of convexity motivate the following approach towards the characterization of f^{qc}. Construct an upper bound $f \geq \tilde{f}$ for the rank-one convex envelope and prove that $\tilde{f}$ is polyconvex. Then necessarily

$$\tilde{f} \geq f^{\mathrm{rc}} \geq f^{\mathrm{pc}} \geq \tilde{f}$$

and hence equality holds throughout this chain of inequalities. We illustrate this process in Section 4.

3 Uniform Bounds on the Deformation Gradient for Functionals with Quadratic Growth

Almost all regularity results in the literature without explicit convexity assumptions rely on strong assumptions on the behavior of the energy densities at infinity. For example, the pioneering work Chipot and Evans (1986) assumes that the density is twice continuously differentiable and that the second derivatives converge to a positive definite matrix at infinity. These assumptions are usually not satisfied for energy densities arising in nonlinear elasticity.

In order to formulate results without such a strong assumption, we restrict our attention to a special class of functionals which are given as the relaxation of the squared distance function to a compact set $K \subset \mathbb{M}^{m\times n}$. That is, let $F_K(\cdot) = \mathrm{dist}^2(\cdot, K)$ denote the squared Euclidean distance and consider

$$I[u] = \int_\Omega F_K^{\mathrm{qc}}(Du)\mathrm{d}y\,. \tag{3}$$

Under the additional assumption that K admits supporting balls of a given fixed radius at each boundary point it was shown in Dolzmann et al. (2011) that the gradient of any minimizer of (3) belongs to $L^\infty_{\mathrm{loc}}(\Omega; \mathbb{M}^{m\times n})$. Moreover, using the results in Fuchs (1997) one can improve this assertion if additional assumptions are made. For example, if $K \subset \mathbb{M}^{2\times 2}$ is a compact and convex subset in the two-dimensional subspace of all conformal matrices, then all extremals of (3) are locally Lipschitz continuous, and even of class $C^{1,\alpha}_{\mathrm{loc}}(\Omega; \mathbb{R}^2)$ for some $\alpha \in (0, 1]$. Note that in all these examples the distance function is convex and therefore the relaxation F_K^{qc} coincides with F_K. If convexity of the set fails, then one cannot expect uniform bounds. The natural replacement for L^∞ is the space BMO of all functions with bounded mean oscillation. In fact, it was show in Dolzmann et al. (2011) that minimizers of (3) lie in this space if K is any compact set in the space of all $m \times n$-matrices. The proof relies on an explicit representation of the relaxation which follows from Ball et al. (2000). A counterexample to uniform bounds is reviewed in Section 4.

4 Relaxation of a One-Well Problem with p-Growth

Let $\operatorname{dist}(X, \mathrm{SO}(2))$ be the Euclidean distance of a matrix $X \in \mathbb{M}^{2\times 2}$ to the set of all proper rotations, that is,

$$F(X) = \operatorname{dist}(X, \mathrm{SO}(2)) = \min_{Q\in \mathrm{SO}(2)} |X - Q| .$$

We write $F_p = F^p$ for the pth power of this function. In view of (1), (2) and $|Q| = \sqrt{2}$ for all $Q \in \mathrm{SO}(2)$ it follows that

$$F_2(X) = \big(|X^+| - \sqrt{2}\big)^2 + |X^-|^2 = 2|X^+|^2 - 2\sqrt{2}|X^+| + 2 - 2\det X = \big(\sqrt{2}|X^+| - 1\big)^2 + 1 - 2\det X .$$

This function is certainly not convex along a direction $t \mapsto tC$ where C is a conformal matrix. Since conformal matrices are not rank-one matrices, the construction of $\tilde f$ as in Section 2 cannot be achieved by an optimization of the energy along conformal directions in matrix space. In order to proceed one notes first that

$$\det(A + B) = \det A + \begin{pmatrix} a_{22} & -a_{21} \\ -a_{12} & a_{11} \end{pmatrix} : \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} + \det B \quad \text{for all } A,\ B \in \mathbb{M}^{2\times 2}$$

and hence the determinant is in fact an affine function along any rank-one line $t \mapsto X + tR$ with $X,\ R \in \mathbb{M}^{2\times 2}$ and $\operatorname{rank} R = 1$. Therefore we may focus on the quadratic term in the energy. We assert that this contribution to the energy can be reduced to zero by a laminate for all $X \in \mathbb{M}^{2\times 2}$ with $|X^+| < 1/\sqrt{2}$. Indeed, let I be the identity matrix in the space of all real 2×2-matrices and choose any vector $a \in \mathbb{R}^2$ with $|a| = 1$ and set $R = a \otimes a^\perp$ where $a^\perp$ denotes the vector which is obtained by rotating a by $\pi/2$ in counterclockwise direction. Then R is a rank-one matrix. Consider the rank-one line $t \mapsto X_t = X(I + tR)$ and the function $t \mapsto \gamma(t) = \sqrt{2}|X_t^+| - 1$ along this line. Then $\gamma(0) < 0$ and the function has linear growth at infinity since the conformal part of any rank-one matrix is different from zero. Hence there exist two parameters $t_\pm$ and corresponding matrices $X_\pm$ such that $t_- < 0 < t_+$ and $\gamma(t_\pm) = 0$. We set $\lambda = t_+/(|t_-| + t_+)$, observe that $X = \lambda X_- + (1 - \lambda)X_+$ and infer in view of the convexity of F_2^{rc} along rank-one directions that

$$F_2^{\mathrm{rc}}(X) \le \lambda F_2^{\mathrm{rc}}(X_-) + (1-\lambda)F_2^{\mathrm{rc}}(X_+) \le \lambda F_2(X_-) + (1-\lambda)F_2(X_+) = 1 - 2\det X . \tag{4}$$

For future reference we observe that F_2 is in fact constant on $\{X_-,\ X_+\}$ since

$$\det X_t = \det\big(X(I + tR)\big) = \det X\ \det\big(I + ta \otimes a^\perp\big) = \det X\ \big(1 + t\langle a, a^\perp\rangle\big) = \det X . \tag{5}$$

This suggests to define

$$\tilde f(X) = \begin{cases} 1 - 2\det X + \big(\sqrt{2}|X^+| - 1\big)^2 & \text{if } |X^+| \ge 1/\sqrt{2}\,, \\ 1 - 2\det X & \text{otherwise,} \end{cases}$$

and it follows $F_2^{\mathrm{qc}} = \tilde f$ if we can prove that $\tilde f$ is polyconvex. However, this follows easily since $\tilde f$ is the sum of the polyconvex function $1 - 2\det X$ and the function $(g \circ h)(X)$ where $g(t) = (\sqrt{2}t - 1)_+^2$ and $h(X) = |X^+|$. Here we write $a_+ = \max\{a, 0\}$ for $a \in \mathbb{R}$. Hence g is convex and monotonically increasing and h is convex. The concatenation of a convex and increasing function with a convex function is again convex and hence $\tilde f$ is the sum of a polyconvex and a convex function, thus polyconvex.

We now review well-known facts in order to state a more general result on the characterization of the semiconvex envelopes of functions. They have been widely used, both in theoretical investigations as well as for algorithmic approaches, see, e.g., Bartels (2004); Bartels et al. (2006); Carstensen and Roubíček (2000); Carstensen (2003); Carstensen et al. (2008); DeSimone and Dolzmann (2002); Dolzmann (1999); Kochmann and Hackl (2011); Kohn and Strang (1986); Kružík and Luskin (2003); Kružík et al. (2005); Pedregal (1997); Roubíček (2002); Šilhavý (2007a) and the references therein. The construction just described is usually referred to as a simple laminate. More generally, $\tilde f$ can be constructed by optimizing in a set of N matrices which satisfy the H_N condition in Dacorogna (1989). Here we say that the pairs $(X_i.\lambda_i)$, $i = 1, \dots, N$, with $X_i \in \mathbb{M}^{m\times n}$ and $\lambda_i \in (0, 1)$, $\lambda_1 + \ldots + \lambda_N = 1$ satisfy the condition H_N if the following is true: For $N = 2$ we have $\operatorname{rank}(X_1 - X_2) = 1$. If $N > 2$, then one can relabel the matrices in such a way that $\operatorname{rank}(X_{N-1} - X_N) = 1$ and such that the pairs (Y_i, μ_i), $i = 1, \dots, N - 1$ with

$$(Y_i, \mu_i) = (X_i, \lambda_i)\,, i = 1, \dots, N - 2,\ \mu_{N-1} = \lambda_{N-1} + \lambda_N\,, Y_{N-1} = \frac{1}{\lambda_{N-1} + \lambda_N}\big(\lambda_{N-1}X_{N-1} + \lambda_N X_N\big)$$

satisfy the H_{N-1} condition. Finally, $X = \lambda_1 X_1 + \ldots + \lambda_N X_N$. Note that this construction implies for a rank-one convex function

$$(\lambda_{N-1} + \lambda_N) f\Big(\frac{\lambda_{N-1}}{\lambda_{N-1}+\lambda_N}\, X_{N-1} + \frac{\lambda_N}{\lambda_{N-1}+\lambda_N}\, X_N \Big) \leq \lambda_{N-1} f(X_{N-1}) + \lambda_N f(X_N)$$

and by induction

$$f(X) \leq f\Big(\sum_{i=1}^N \lambda_i X_i \Big)\,. \tag{6}$$

It is natural to identify this set of matrices with measures, called finite laminates, and to define integration of a continuous function with respect to such a measure ν by

$$\nu = \sum_{i=1}^N \lambda_i \delta_{X_i}\,, \qquad \langle \nu, f \rangle = \sum_{i=1}^N \lambda_i f(X_i)\,, \qquad \langle \nu, id \rangle = \sum_{i=1}^N \lambda_i X_i = X\,.$$

The calculation which led to (4) can be extended to finite laminates and yields

$$\langle \nu, f \rangle = \sum_{i=1}^N \lambda_i f(X_i) \geq \sum_{i=1}^N \lambda_i f^{\rm rc}(X_i) \geq f^{\rm rc}\Big(\sum_{i=1}^N \lambda_i X_i \Big) = f^{\rm rc}(X)\,. \tag{7}$$

Note that each ν is by construction a probability measure. As pointed out by Müller and Šverák (1999), the minimization can be performed in the larger class of measures which are obtained as the weak-$*$ closure of finite laminates with support in a compact set K which we will refer to as generalized constructions or laminates $\nu \in \mathcal{M}^{\rm rc}(K,X)$ with center of mass X. That is, for every $\nu \in \mathcal{M}^{\rm rc}(K,X)$ there exists a sequence ν_k of finite laminates with support in K such that for all continuous functions f the identity

$$\langle \nu, f \rangle = \lim_{k\to\infty} \langle \nu_k, f \rangle$$

holds true. In particular, for $f \equiv 1$ one obtains that ν is a probability measure. Moreover, if f is rank-one convex, then (6) implies that

$$\langle \nu, f \rangle = \lim_{k\to\infty} \langle \nu_k, f \rangle \geq f(X)\,. \tag{8}$$

However, if f is any continuous function, then $\langle \nu, f \rangle \geq f^{\rm rc}(X)$ for all finite laminates in $\mathcal{M}^{\rm rc}(K,X)$, see (7), and the same assertion holds true for all laminates,

$$\langle \nu, f \rangle \geq f^{\rm rc}(X) \qquad \text{for all } \nu \in \mathcal{M}^{\rm rc}(K,X)\,. \tag{9}$$

After these preparations we are in a position to state a principle of stability under exponentiation in the convex case. Suppose that $f\colon \mathbb{M}^{m\times n} \to [0,\infty)$ is a function with $f^{\rm pc} = f^{\rm qc} = f^{\rm rc}$ and that there exists for all $X \in \mathbb{M}^{m\times n}$ a compact set K and a generalized construction $\nu \in \mathcal{M}^{\rm rc}(K,X)$ with the following properties:

(a) the center of mass is the given matrix X, i.e., $\langle \nu, id \rangle = X$;

(b) the generalized construction realizes the infimum of the energy, i.e., $f^{\rm rc}(X) = \langle \nu, f \rangle$;

(c) f is constant on the support $\mathrm{supp}(\nu)$.

Then the relaxation of f^p, $p \geq 1$, is given by $(f^{\rm qc})^p$. In order to verify the assertion we observe that the natural candidate for the function $\tilde{f}$ is given by $\tilde{f} = (f^{\rm rc})^p$. Clearly $f^p \geq (f^{\rm rc})^p$ and in view of assumptions (b) and (c),

$$\begin{aligned} \tilde{f}(X) = (f^{\rm rc})^p(X) \ &= \langle \nu, f \rangle^p = \Big(\int_{\mathbb{M}^{m\times n}} f(A) \mathrm{d}\nu(A) \Big)^p = \big(f\big|_{\mathrm{supp}\,\nu} \big)^p \Big(\int_{\mathbb{M}^{m\times n}} \mathrm{d}\nu(A) \Big)^p \\ &= \int_{\mathbb{M}^{m\times n}} f^p(A) \mathrm{d}\nu(A) = \langle \nu, f^p \rangle \geq (f^p)^{\rm rc}(X)\,. \end{aligned}$$

It remains to prove that $\tilde{f}$ is polyconvex. Since $f^{\rm rc} = f^{\rm pc}$, there exists a convex function g which depends only on the vector $T(X)$ of all minors of X such that $f^{\rm rc}(X) = g(T(X))$. Since f is nonnegative we conclude the same for g and hence $(f^{\rm rc})^p(X) = (h \circ g)(T(X))$ where $h(t) = t_+^p$ is a convex and nondecreasing function. Therefore $h \circ g$ is convex and $(h \circ g)(T(X))$ is a polyconvex function in X. The arguments in Section 2 imply that $\tilde{f}$ is the relaxation of f^p and that $(f^p)^{\rm rc} = (f^p)^{\rm qc} = (f^p)^{\rm pc}$.

We now return to the specific example $F_p = \mathrm{dist}^p(\cdot, \mathrm{SO}(2))$. The construction for $f^{\rm rc}$ in X is based on a finite laminate $\nu = \lambda\delta_{X_+} + (1-\lambda)\delta_{X_-}$ and on the support of ν the function f coincides with the constant function $Y \mapsto 1 - 2\det X$, see (5). Hence we obtain from the foregoing discussion, that

$$F_p^{\rm rc}(X) = F_p^{\rm qc}(X) = F_p^{\rm pc}(X) = \left(F_2^{\rm rc}(X)\right)^{p/2} = \begin{cases} \mathrm{dist}^p(X, \mathrm{SO}(2)) & \text{if } |X^+| \geq 1/\sqrt{2}\,, \\ (1 - 2\det X)^{p/2} & \text{otherwise,} \end{cases} \qquad p \geq 2\,. \quad (10)$$

This representation is very convenient for the subsequent discussion of minimizers with unbounded gradients. The first formula for the relaxation of F_p can be found in Šilhavý (2001, 2007b) where general isotropic functions are considered and a formula in terms of the singular values is presented.

We finally present an unbounded minimizer for the corresponding quadratic variational problem following Dolzmann et al. (2011). Let $\Omega = B(0,1)$ be the unit disk in the plane. Minimize in $W_0^{1,2}(\Omega; \mathbb{R}^2)$ the energy

$$\int_\Omega F_2^{\rm qc}(\nabla u)\mathrm{d}x\,.$$

We assert that $u(x,y) = \frac{1}{2}(x,-y)\ln\left(x^2+y^2\right)$ is a minimizer. Note that this function appears already in Iwaniec (1986). The function u satisfies

$$Du(x,y) = \frac{1}{2}\left(\ln(r^2)+1\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{1}{2r^2}\begin{pmatrix} x^2-y^2 & 2xy \\ -2xy & x^2-y^2 \end{pmatrix}$$

where $r^2 = x^2 + y^2$. Thus we have $|Du^+| = 1/\sqrt{2}$ a.e. on Ω and hence $F_2^{\rm qc}(Du) = 1 - 2\det Du$ on Ω. Let $\phi \in W_0^{1,2}(\Omega;\mathbb{R}^2)$ and observe that

$$\int_\Omega F_2^{\rm qc}(Du + D\phi)\mathrm{d}y \geq \int_\Omega \left(1 - 2\det(Du + D\phi)\right)\mathrm{d}y = \int_\Omega \left(1 - 2\det Du\right)\mathrm{d}y = \int_\Omega F_2^{\rm qc}(Du)\mathrm{d}y.$$

This chain of inequalities verifies that u is in fact a minimizer of the functional.

5 Conclusion

We presented sufficient conditions for uniform bounds on the deformation gradient and provided an example with a logarithmic divergence which shows that the assertions are optimal. It is a natural question whether the counterexample in Section 4 can be extended from the quadratic case to the p-growth case. This remains a challenging problem, but it seems that the representation (10) could provide a link between the quadratic and the superquadratic case that could help to settle this demanding problem.

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