Some Remarks on Quasiconvexity, Inner Variations, and Optimal Meshes

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Received: March 12, 2007 Revised manuscript received: December 3, 2007

We explore a formulation of quasiconvexity in terms of inner variations instead of variations of the dependent variable. This leads to a specific transformation of integrands that is stable for rank-one convexity, quasiconvexity, and polyconvexity, but not for convexity. An interesting application of these ideas is concerned with the analysis of optimal adaptive meshes for variational problems. This theme is not new either in the analytical or numerical treatment. We complete the discussion with some easy examples in dimension one, and defer the much more complex situation in higher dimension for a later work. An interesting point is that our remarks are valid when the number of components for fields is not greater than the number of independent variables.

Keywords: Inner variations, multiplicative quasiconvexity, adaptivity

1991 Mathematics Subject Classification: 49J45

1. Introduction

Let us consider a variational problem (P) of the type

Minimize in
$$u$$
: $I(u) = \int_{\Omega} \phi(x, \nabla u(x)) dx$

where u is taken in a certain Sobolev space dictated by the growth properties of the integrand $\phi: \mathbf{M}^{m \times N} \to \mathbf{R}$

$$c(x)|A|^p-1 \leq \phi(x,A) \leq C(|A|^p+1), \quad 1$$

Feasible fields u are thus taken in $W^{1,p}(\Omega; \mathbb{R}^m)$ and they comply with a Dirichlet boundary condition $u = u_0$ on $\partial\Omega$. Ω is a bounded, regular domain in \mathbb{R}^N . If ϕ is quasiconvex (convex if m = 1 or N = 1) in A for a.e. $x \in \Omega$, then it is well-known ([1], [8]) that there are (global) minimizers for the variational problem, but for p in a certain range (p < N) or where the coercivity coefficient c(x) vanishes, such minimizers may fail to be regular or may present regions of high concentration to the point that sometimes they may even fail to be continuous. The numerical approximation of such minimizers poses a real challenge as good approximations would require very fine meshes in such regions. When such convexity conditions do not hold the situation is even more dramatic (see

*Supported by project MTM2004-07114 from Ministerio de Educación y Ciencia (Spain) and by project PAI05-029 from JCCM (Castilla-La Mancha).

ISSN 0944-6532 / \$ 2.50 © Heldermann Verlag

for example [5], [6], [15]). Our purpose is to build into the variational problem flexible meshes as part of the minimization process, and this will lead us to talk about inner variations, and quasiconvexity in a multiplicative form. Until the final section on the examples, we will drop the explicit x dependence of ϕ as it will be essentially irrelevant in our arguments.

Suppose $v : \Omega \to \Omega$ is a genuine change of variables in Ω , i.e., $v \in W^{1,\infty}(\Omega; \mathbf{R}^N)$, v is one-to-one so that det $\nabla v > 0$ a.e. $x \in \Omega$, and v(x) = x on $\partial\Omega$. If u is feasible for (P), so is the composition $U(x) = u(v^{-1}(x))$, and after performing the change of variables

$$\int_{\Omega} \phi(\nabla U(x)) \, dx = \int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) \, dx.$$

Consider u as being given. The minimization problem

Minimize in
$$v$$
: $J(v) = \int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) dx$

under the conditions just indicated on v, would furnish the "best mesh for u". This phylosophy has already been treated and studied both from a analytical and numerical point of view ([11], [14]). Apparently, it enjoys a long-established tradition (see references in [14]).

From an analytical point of view, a fundamental issue is whether this optimization problem does indeed admit optimal solutions. As it is well-known, this amounts to being able to apply the direct method of the Calculus of Variations to this minimization problem. A main ingredient is the quasiconvexity of the integrand

$$\varphi : \mathbf{M}^{N \times N} \to \mathbf{R}, \quad \varphi(X) = \phi(AX^{-1}) \det X$$

for any given $A \in \mathbf{M}^{m \times N}$. This is essentially a problem in non-linear elasticity ([1], [7]). We will show that the process $\phi \mapsto \varphi$ is an involution on the class of polyconvex, quasiconvex, and rank-one convex integrands, but it is clear that it is not so on the class of convex densities.

Even further, we can consider the full minimization problem (CP)

Minimize in
$$(u, v)$$
: $H(u, v) = \int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) dx$

for u and v as above. This sort of variational problems are reminiscent of problems of variation of domains examined in the context of certain models in defective crystals ([10]) involving variation of the domain ([9]). A main issue here is the quasiconvexity of the integrand

$$\psi : \mathbf{M}^{m \times N} \times \mathbf{M}^{N \times N} \to \mathbf{R}, \quad \psi(A, X) = \phi(AX^{-1}) \det X.$$

We will show that this is the case too, and analyze this problem.

From the point of view of approximations, the whole issue is that if we consider discrete versions of both problems (P) and (CP), by restricting feasibility to appropriate finite dimensional spaces V_k , then in order to capture fine features of the minimizer for (P) one would need very fine meshes that most likely would be useless in vast regions of Ω while

for (CP) this will not be the case as the discretization of the variables in v would focus on critical zones for the minimizers as it is typical in adaptivity. In this way adaptability is built into the problem itself. This is however a very delicate issue as it is known that invertibility may not be preserved by projection onto finite dimensional subspaces (see [4]). A way to avoid these difficulties is to restrict attention to changes of variables v which are "homotopic" to the identity in the sense that v can be attained by a continuous family of changes of variables starting from the identity. If v is thought of as a discrete, piecewise affine mesh, then it will be feasible if it represents a mesh that can be continuously deformed, preserving the injectivity, to the identity.

Though a main motivation for our remarks is the treatment of optimal meshes, our remarks in Sections 2 and 3 also have some analytical significance for vector problems in the Calculus of Variations, and they may be taken as a preparation for the main part in Section 4.

We end up with some easy examples to emphasize these issues.

2. Quasiconvexity

We are used to define quasiconvexity in a "additive" way. A function $\phi : \mathbf{M}^{m \times N} \to \mathbf{R}$ is said to be quasiconvex in a matrix F if

$$\phi(F) \leq \int_D \phi(F + \nabla u(x)) \, dx$$

for any unitary, Lipschitz domain $D \subset \mathbf{R}^N$ (|D| = 1), and any test field $u : D \to \mathbf{R}^m$ such that u = 0 on ∂D . These are variations of the dependent variable. This concept also admits a "multiplicative" version (when $m \leq N$) which requires the use of innervariations, variations with respect to the independent variables ([12]).

Lemma 2.1. If $m \leq N$, the integrand ϕ is quasiconvex at F if and only if

$$\phi(F) \le \int_D \phi(F\nabla v(x)) \, dx$$

for any test field $v: D \to \mathbf{R}^N$ such that v(x) = x on ∂D .

Proof. If $N \ge m$, let F be a matrix for which another matrix F' can be found so that FF' = identity of size $m \times m$.

Let u be any field for which we can test quasiconvexity for ϕ , i.e., u is smooth and u(x) = 0over ∂D . Define the field $v : D \to \mathbf{R}^N$ by putting v(x) = x + F'u(x). Then it is clear that v(x) = x on ∂D , and

$$F\nabla v(x) = F + FF'\nabla u(x) = F + \nabla u(x).$$

On the other hand, if v(x) = x on ∂D , then we can take u(x) = F(v(x) - x) so that $F + \nabla u(x) = F \nabla v(x)$.

Since the set of matrices F for which we can find such a matrix F' so that FF' = identity is dense, the proof is finished.

We will assume henceforth $N \ge m$, without further indication.

Suppose now that the test field v is a true change of variables in D not affecting the boundary ∂D (v(x) = x on ∂D), and so is v^{-1} . Then

$$\int_D \phi(F\nabla v^{-1}(x)) \, dx = \int_D \phi(F\nabla v(y)^{-1}) \det \nabla v(y) \, dy.$$

If ϕ is quasiconvex, then by the previous lemma,

$$\phi(F) \leq \int_D \phi(F \nabla v(y)^{-1}) \det \nabla v(y) \, dy$$

for any such test field v. This justifies the following proposition.

Proposition 2.2. If $\phi : \mathbf{M}^{m \times N} \to \mathbf{R}$ is quasiconvex, then

$$\varphi : \mathbf{M}^{N \times N}_{+} \to \mathbf{R}, \quad \varphi(X) = \det X \, \phi(FX^{-1})$$

is quasiconvex for any matrix F.

Here $\mathbf{M}^{N \times N}_{+}$ indicates the set of non-singular matrices with positive determinant.

Proof. The proof has just been indicated. Notice that if $v: D \to D$ is locally invertible because det $\nabla v(x) > 0$ for a.e. $x \in \Omega$, then due to the fact that v(x) = x over ∂D , v is indeed globally injective, i.e. a global change of variables in D. See [2].

By our multiplicative version of quasiconvexity Lemma 2.1, we have to show that for a test field v as the one in the preceding paragraph, we have the appropriate inequality. But since v is a global change of variables, then we have just checked the inequality before the statement of the proposition. Note that it suffices to check quasiconvexity at the identity matrix.

Notice that if we define the functional transformation T by putting (F =identity)

$$T\phi(X) = \det X \phi(X^{-1})$$

then $T(T\phi) = \phi$. In general, we put $T_F\phi(X) = \det X\phi(FX^{-1})$.

What is the behavior of this transformation for convexity, polyconvexity, and rank-one convexity? It is obvious that convexity is not preserved under T. However, it is elementary to check that polyconvexity and rank-one convexity are indeed conserved.

Remark 2.3. If ϕ is polyconvex, respectively rank-one convex, so is $T_F \phi$ for any F.

Notice that the transformation T_F preserves null-lagrangians since Lemma 2.1 is also valid when we replace that family of inequalities by the corresponding equalities.

Concerning rank-one convexity, it is easy to realize that if two square matrices F_1 and F_2 are rank-one related so are det $F_1FF_1^{-1}$ and det $F_2FF_2^{-1}$. Recall that for a non-singular matrix A, $A^{-1} = (1/\det A) \operatorname{adj} A^T$.

This transformation also says something about gradient Young measures.

Remark 2.4. Let ν be a (homogeneous) gradient Young measure supported in $\mathbf{M}^{N \times N}_{+}$. Then the probability measure $T\nu$ defined through

$$\langle \varphi, T\nu \rangle = \frac{1}{\int_{\mathbf{M}^{N \times N}} \det A \, d\nu(A)} \int_{\mathbf{M}^{N \times N}} \varphi(A^{-1}) \det A \, d\nu(A)$$

is also a gradient Young measure.

3. Non-linear elasticity

Let us focus in this section on the particular case of non-linear elasticity where we have

$$\phi : \mathbf{M}^{N \times N} \to \mathbf{R}, \quad \phi(X) = +\infty \text{ if } \det X \le 0,$$

and ϕ verifies other physically relevant restrictions. We can incorporate into the variational principle of minimal energy both variations of the dependent and independent variables. This leads us to consider

Minimize in
$$(u, v)$$
: $I(u, v) = \int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) dx$

subject to the constraints

$$(u,v) \in W^{1,p}(\Omega; \mathbf{R}^N) \times W^{1,\infty}(\Omega; \mathbf{R}^N), u(x) = u_0(x), v(x) = x, \text{ on } \partial\Omega,$$

and both u and v are one-to-one mappings. This form of variational principles reminds us of variation of the domain ([9]), though here we are not enforcing the incompresibility restriction det $\nabla v(x) = 1$ and, on the other hand, we have a very precise boundary condition for v.

Proposition 3.1. Let $\overline{\phi}(X,Y) = \det Y\phi(XY^{-1})$, for $(X,Y) \in \mathbf{M}^{2N \times N}$. If ϕ is quasiconvex at F, so is $\overline{\phi}$ at (F, identity).

Proof. The proof is nothing but redoing the previous computations with the composition $u \cdot v^{-1}$, where u and v have affine boundary values given by F and identity, respectively. Namely

$$\int_D \phi(\nabla u \cdot v^{-1}(x)) \, dx = \int_D \phi(\nabla u(y) \nabla v(y)^{-1} \det \nabla v(y) \, dy.$$

This quantity is

$$\int_D \overline{\phi}(\nabla u(x), \nabla v(x)) \, dx$$

while $\phi(F) = \overline{\phi}(F, \text{ identity})$. Hence, from the quasiconvesity of ϕ at F we conclude the quasiconvexity of $\overline{\phi}$ at (F, identity).

The advantage of looking at variational problems in this way is that we have more variables (u, v) and, especially for non-convex problems, this might furnish better approximations as we have more ways to escape local minima.

4. Optimal adaptive meshes

This is the same as in the non-linear elasticity setting, but this time the mapping u could have any number of components

$$I(u,v) = \int_{\Omega} \phi(\nabla u(x)\nabla v(x)^{-1}) \det \nabla v(x) \, dx$$

where $u \in W^{1,p}(\Omega; \mathbf{R}^m)$, $v \in W^{1,\infty}(\Omega; \mathbf{R}^N)$, $u = u_0$ and v(x) = x on $\partial\Omega$. Here the mapping v accounts for the adaptivity of the mesh, and it is done in such a way as to minimize the energy. At the same time, the flexibility attached to v may help in escaping local minima phenomena.

We look at the energy above for fixed u, regarded as a good approximation to the minimizer of the problem

Minimize in
$$u$$
: $\int_{\Omega} \phi(\nabla u(x)) dx$

for $u \in W^{1,p}(\Omega; \mathbf{R}^m)$, $u = u_0$ on $\partial\Omega$. We place ourselves in the typical main assumption to apply the direct method of the Calculus of Variations to this problem ([8]):

• the density $\phi : \mathbf{M}^{m \times N} \to \mathbf{R}$ is quasiconvex (convex if m = 1) and

$$c|A|^p - 1 \le \phi(A) \le C(|A|^p + 1), \quad 0 < c < C, p > 1.$$

It is well-known that under this hypothesis, we have minimizers for this variational problem. If, in addition, ϕ is strictly convex, the minimizer is unique. Moreover if we assume further regularity (smoothness) on ϕ , such minimizer will be a weak solution of the associated Euler-Lagrange equation or system

div
$$\left[\frac{\partial \phi}{\partial A}(\nabla u(x))\right] = 0$$
 in Ω , $u = u_0$ on $\partial \Omega$.

Suppose now that u is not the exact minimizer of our problem, i.e. not the exact solution of the Euler-Lagrange problem, but a reasonably good approximation. We would now like to find the best mesh for it, in the sense that we want the mesh to adapt itself to the approximation u already found (probably by using another initial mesh). Since in this situation the field u is fixed, we can allow the exponent p to be 1 as well.

Theorem 4.1. Suppose that $u: \Omega \subset \mathbf{R}^N \to \mathbf{R}^m$ is a given field in $W^{1,p}(\Omega; \mathbf{R}^m)$ so that

$$\int_{\Omega} \phi(\nabla u(x)) \, dx < +\infty,$$

for a quasiconvex integrand ϕ as above with $p \ge 1$. Then for each constant M > 0, the variational problem

Minimize in
$$v \in \mathcal{A}_M$$
: $\int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) dx$

where

$$\mathcal{A}_M = \left\{ v \in W^{1,\infty}(\Omega; \mathbf{R}^N) : v(x) = x \text{ on } \partial\Omega, \det \nabla v(x) > 0, \|\nabla v^{-1}\|_{W^{1,\infty}(\Omega; \mathbf{R}^N)} \le M \right\},$$

admits a minimizer.

Proof. The proof is simple after our remarks in Section 2. Consider the integrand

$$\varphi: \Omega \times \mathbf{M}^{N \times N}_{+} \to \mathbf{R}, \quad \varphi(x, X) = \phi(\nabla u(x) X^{-1}) \det X.$$

By Proposition 2.2, because ϕ is quasiconvex, this new integrand is quasiconvex for a.e. $x \in \Omega$. So therefore the integrand associated with it in the statement of the theorem is weak lower semicontinuous (see [3], [8]) in $W^{1,\infty}(\Omega; \mathbf{R}^N)$. This is standard.

For each M, the set of admissibility \mathcal{A}_M is weakly * closed in $W^{1,\infty}(\Omega; \mathbf{R}^N)$. In addition, for a minimizing sequence v_j of changes of variables, we have a change of variables v which is a weak limit in $W^{1,\infty}(\Omega; \mathbf{R}^N)$ of v_j . Hence by weak lower semicontinuity, we conclude that

$$\int_{\Omega} \phi(\nabla u(x)\nabla v^{-1})(x)) \det \nabla v(x) \, dx \le \liminf_{j \to \infty} \int_{\Omega} \phi(\nabla u(x)\nabla v_j(x)^{-1}) \det \nabla v_j(x) \, dx.$$

We deduce that v is a minimizer for our problem.

When looking for a version of this result that allows explicit dependence of ϕ on x and u, notice that by the usual change of variables

$$\int_{\Omega} \phi(x, u \cdot v^{-1}(x), \nabla(u \cdot v^{-1})(x)) \, dx = \int_{\Omega} \phi(v(y), u(y), \nabla u(y) \nabla v(y)^{-1}) \det \nabla v(y) \, dy.$$

This would require in principle continuous dependence of ϕ both on x and on u, contrary to the usual requirement of only measurability with respect to x. This however is not a problem from the practical point of view, because the transformation v carries null sets over null sets and hence the integrand on the right-hand side is well-defined even under just measurability with respect to x.

One final important remark is that once the optimal mesh v has been found for u, the optimal map is the composition $u \cdot v^{-1}$. This is like saying that if u was found by using a certain triangulation τ , the optimal mesh for u is the deformed triangulation $v(\tau)$. In other words, take the range of u defined over the new deformed triangulation $v(\tau)$.

From a more practical point of view, one is led to consider the process by which, starting out with v = identity, one finds the optimal mesh for a given u. In this sense, changes of variables (or meshes at the discrete level) are only allowed if they are homotopic to the identity.

In this regard, we can say that a change of variables $v : \Omega \to \Omega$, one-to-one, Lipschitz, such that v(x) = x for $x \in \partial \Omega$ is homotopic to the identity if there is $V(t, x) : [0, 1] \times \Omega \to \Omega$, continuous and Lipschitz in x such that

$$V(0,x) = x$$
, $V(1,x) = v(x)$, $V(t,x) = x$ for $x \in \partial \Omega$,

and each $V(t, \cdot)$ is one-to-one.

In a natural way, this homotopy V is supposed to decrease energy as "time" t proceeds. Indeed, one can try to get this homotopy from the gradient flow of the functional

$$J(v) = \int_{\Omega} \phi(\nabla u(x) \nabla v(x)^{-1}) \det \nabla v(x) \, dx$$

for fixed u. This would lead to consider the parabolic system

$$V_t(t,x) - \operatorname{div}\left[\frac{\partial\psi}{\partial A}(x,\nabla V(t,x)\right] = 0 \quad \text{in } (0,+\infty) \times \Omega, \tag{1}$$

under boundary conditions V(t, x) = x for $x \in \partial \Omega$ for all time, and initial conditions V(0, x) = x. Here

$$\psi(x,A) = \phi(\nabla u(x)A^{-1}) \det A.$$

As far as we know, not much is known in this great generality for such a parabolic system of partial differential equations especially when ϕ is quasiconvex but not convex. Even in dimension one, these parabolic problems have an impressive appearance because of the inhomogeneity coming from u and the ocurrence of the inverse A^{-1} in ψ .

5. Some examples in dimension one

It is not easy to work out explicit examples analytically in dimension higher than one, because that amounts to solving a system of partial differential equations, typically nonlinear. For this reason we will restrict attention here just to the one-dimensional situation.

Consider first the very simple example

$$u: (0,1) \to \mathbf{R}, \quad u''(x) = 0 \text{ in } (0,1), \quad u(x) = x \text{ on } \{0,1\}.$$

It is obvious that the solution is in fact u(x) = x which is the minimizer of the functional

$$\int_0^1 |u'(x)|^2 \, dx$$

subject to u(x) = x on the end-points x = 0 and x = 1.

Let u(x) be any admissible field for this problem, and consider the variational problem determining the best mesh for such u. In this very simple situation, we realize that we are seeking the minimizer of the functional

$$\int_0^1 \frac{u'(x)^2}{v'(x)} \, dx$$

subject to v(0) = 0, v(1) = 1 and v'(x) > 0. If we overlook the positivity of the derivative and proceed to find the optimal v by using the associated Euler-Lagrange equation, it is elementary to find, after some easy manipulations, that

$$v(x) = \frac{1}{\int_0^1 |u'(y)| \, dy} \int_0^x |u'(y)| \, dy.$$

We always have positive derivative provided u' never vanishes, or it does in a negligible set. Notice that if u' > 0 then u = v, and so the composition $u \cdot v^{-1}$ always furnishes the true minimizer of the original problem. However, if, for example u(x) = x(5-4x), which is not monotone, then one can easily obtain that

$$v(x) = \begin{cases} 8u(x)/17, & 0 \le x \le 5/8, \\ (25 - 8u(x))/17, & 5/8 \le x \le 1. \end{cases}$$



Figure 5.1: Exact computations.

Both v and the composition $u \cdot v^{-1}$ are drawn in Figure 5.1. We can easily argue that this time the mapping v we have got is not a minimizer as the minimizer would exhibit a concentration effect near the left end-point. If we go through some elementary simulations for this same example with meshes of 5, 7 and 11 elements, we obtain the pictures shown in Figure 5.2, respectively.

If we use as a starting approximation, functions whose range are the same as that of the exact minimizer like $u(x) = \sqrt{x}$ or $u(x) = x^2$, then the computations yield the exact minimizer. See Figure 5.3.

The corresponding parabolic problems described at the end of the last section are of the type

$$V_t(t,x) + \frac{d}{dx} \left(\frac{u'(x)^2}{V_x(t,x)^2} \right)$$
 in $(0, +\infty) \times (0, 1)$.

Even for simple choices of u, these equations look intimidating.

Our second example is a very simple case of a phenomenon of concentration where the slope of the sought field becomes $+\infty$ in a certain point. Namely, we seek to

Minimize in
$$u$$
: $\int_0^1 \frac{1}{2} (x - \frac{1}{2})^2 u'(x)^2 dx$

subject to $u \in H^1(0,1)$, u(x) = x for $x \in \{0,1\}$. In this situation, the coercivity degenerates at the middle point x = 1/2, and this leads to an infinite slope of the minimizer in this point: the minimizer breaks continuity at this point. If we pretend to capture this phenomenon with regular meshes, it would require very fine meshes indeed. However, if we take u(x) = x, the starting approximation, and simulate the minimizer of the problem

Minimize in
$$v$$
: $\int_0^1 \frac{1}{2} (v(y) - \frac{1}{2})^2 \frac{1}{v'(y)} dy$

subject to v(y) = y for $y \in \{0, 1\}, v' > 0$, then we get surprisingly good results even for



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Figure 5.2: Simulations with meshes of 5, 7, and 11 elements.

rather very coarse meshes. In Figure 5.4, we can see such simulations for meshes of 3, 5, and 7 elements.

We finally consider the typical non-convex Bolza problem with two potential wells at the points ± 1

Minimize in
$$u$$
: $\int_0^1 [(u'(x)^2 - 1)^2 + u(x)^2] dx$

subject to vanishing boundary conditions at both end-points. It is well-known that this simple problem is often used as a paradigmatic situation for the persistence of oscillations (in the derivative) ([5], [6]). Notice how minimizing sequences need to change abruptly and frequently between slopes +1 and -1 to lead the cost to zero.

It is pretty clear by now that persistent oscillations cannot be created by using algorithms based on diffusive (convex) principles, at least for fixed, given meshes. Allowing variations of the independent variable as well, even though it may not fully solve the difficulty of non-convexity, at least it experimentally allows for more ways to create those oscillations. Indeed, we show here some simple numerical simulations with 4, 10, and 20 elements. They are shown in Figure 5.5. We started the simulation from the function identically



Figure 5.3: Simulations for $u(x) = \sqrt{x}$ and $u(x) = x^2$, respectively.



Figure 5.4: Simulations for a minimizer with concentration of the slope at the middle point.

zero on the interval. So we see that the flexibility of permitting to optimize on independent variables as well may be a good alternative for non-convex variational problems.



Figure 5.5: Simulations for the Bolza problem.

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