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From a Nonlinear, Nonconvex Variational Problem to a Linear, Convex Formulation*

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Abstract. We propose a general approach to deal with nonlinear, nonconvex variational problems based on a reformulation of the problem resulting in an optimization problem with linear cost functional and convex constraints. As a first step we explicitly explore these ideas to some one-dimensional variational problems and obtain specific conclusions of an analytical and numerical nature.

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1. Introduction

Nonlinear, nonconvex variational problems have lately received much attention because the behavior of such problems seems apparently connected to the explanation of many situations in science and technology. We are referring to the oscillatory behavior

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inherently associated to lack of convexity. Since there are many papers focused on this issue, we do not discuss it here. We simply mention the importance of these ideas in the understanding of nonlinear elasticity from an energetic viewpoint (see [2]). Our contribution in this paper is to start the analysis of a general treatment of nonconvex variational problems by appropriately transforming a generalized formulation. It turns out that the structure of this new, equivalent variational principle is as regular as one would desire for treatment within the set of classical techniques in optimization theory, both from an analytical and a numerical viewpoint. We show how this formalism yields nontrivial, explicit results of both kinds in a simplified situation.

Our starting point is a typical variational problem in the Calculus of Variations where we seek to minimize the functional

$$I(u) = \int_\Omega f(x, u(x), \nabla u(x))\, dx$$

under appropriate boundary conditions, and possibly under additional restrictions. Since these are not relevant to our discussion we do not specify them. $\Omega \subset \mathbf{R}^N$ is an open, regular, bounded set; $u\colon\ \Omega \to \mathbf{R}^m$ is a deformation belonging to some Sobolev space; and $f\colon\ \Omega \times \mathbf{R}^m \times \mathbf{M}^{m\times N} \to \mathbf{R}$ is a density satisfying suitable technical assumptions that are not important to clarify at this point. It is known that regardless of the convexity properties of f with respect to ∇u, this variational problem is equivalent to a generalized formulation in terms of gradient Young measures [9]. The basic feature of this formulation we would like to stress is the form of the functional itself, overlooking again additional restrictions. Indeed,

$$\tilde{I}(\nu) = \int_\Omega \langle f(x, u(x), \cdot), \nu_x \rangle\, dx$$

is the new functional to be minimized on competing gradient Young measures $\nu = \{\nu_x\}_{x\in\Omega}$. Notice that in this passage we have gone from a nonlinear dependence on functions on ∇u to a linear dependence on more complicated objects ν. The idea we would like to explore is whether it might be possible to go back to an equivalent, variational principle on functions while at the same time retaining linear dependence. Formally, we can do so by using some sort of Parseval's identity with respect to some unspecified, appropriate integral transformation for measures

$$\langle \varphi, \mu \rangle = \int \hat{\varphi}(\xi)\hat{\mu}(\xi)\, d\xi.$$

Applying this basic identity to our generalized functional, we formally obtain

$$\begin{aligned}\int_\Omega \langle f(x, u(x), \cdot), \nu_x \rangle\, dx &= \int_\Omega \int \hat{f}(x, u(x), \cdot)\hat{\nu}_x\, d\xi\, dx\\ &= \int_\Omega \int F(x, u(x), \xi)\hat{\nu}(\xi, x)\, d\xi\, dx.\end{aligned}$$

Thus, we are back to an optimization problem involving functions $\hat{\nu}(\xi, x)$. The important issue is to understand the structure of the set of feasible functions

$$\Lambda = \{\hat{\nu}(\xi, x)\colon\ \nu \text{ admissible for } \tilde{I}\}.$$

Our new, equivalent formulation would read

$$\hat{I}(g) = \int_\Omega \int F(x, u(x), \xi) g(x, \xi)\, d\xi\, dx,$$
$$g \in \Lambda + \text{relationship between } u \text{ and } g,$$

and possibly further constraints inherited by initial restrictions.

In this way we have gained two important features with respect to the initial optimization problem: linear dependence on competing functions, and convexity of the set Λ. On the contrary, one would have to overcome technical difficulties in order to establish rigorously the equivalence of the new variational problem and the original one; more importantly if we pursue a better understanding of optimal behavior, we need an explicit characterization of the set Λ without any reference to measures. We show how this program can be carried out in some simplified, one-dimensional situations where technicalities can be kept to a minimum. In particular, we have an explicit characterization of the set Λ, and show how this explicit information may be utilized to deduce interesting, nontrivial information about optimal behavior.

We consider the scalar, one-dimensional variational problem

$$\text{Minimize} \quad I(u) = \int_a^b \varphi(x, u(x), u'(x))\, dx, \qquad u(a) = A, u(b) = B,$$

where u is supposed to be continuous, belonging to the Sobolev space $W^{1,1}(a, b)$. The integrand φ: $(a, b) \times \mathbf{R} \times \mathbf{R} \to \mathbf{R}$ is assumed to be a Carathéodory function, which means it is continuous on the pair (u, u'), and measurable in x. Furthermore, uniform bounds of the type

$$c(|\lambda|^p - 1) \leq \varphi(x, u, \lambda) \leq C(|\lambda|^p + 1), \qquad p > 1, \tag{1.1}$$

are also assumed on φ. When the dependece of φ on λ is convex for a.e. pair (x, u), the above variational problem admits minimizers, and their existence is shown via the direct method of the Calculus of Variations [4], [9]. However, when such dependence is not convex, oscillatory behavior is typically the outcome, so that minimizing sequences are forced to oscillate on smaller and smaller spatial scales: the more rapidly the oscillation takes place, the smaller the value taken on by the integral. This phenomenon is by now very well-understood as pointed out above. Even further, we restrict attention to

$$\varphi(x, u, \lambda) = \sum_{j=0}^{2n} a_j(x, u)\lambda^j, \qquad a_{2n} \equiv 1,$$

because in this case the transformation from measures to functions materializes, without any trouble, in the moments of underlying Young measures as we will see. We can then use classical results on the characterization of vectors of moments of probability measures in order to write down a fully explicit definition of Λ (Section 2), which in turn will lead us to find interesting analytical and numerical results (Sections 3 and 4, respectively).

2. The Method in the One-Dimensional Case

We take from now on

$$\varphi(x, u, \lambda) = \sum_{j=0}^{2n} a_j(x, u)\lambda^j, \qquad a_{2n} \equiv 1,$$

a monic, even-degree polynomial on λ with coefficients depending on (x, u). We also work without loss of generality on the interval (0, 1) and take admissible, boundary values to be

$$u(0) = u_0, \qquad u(1) = u_1,$$

so that we would like to understand the variational principle

$$\text{Minimize} \quad I(u) = \int_0^1 \sum_{j=0}^{2n} a_j(x, u)(u'(x))^j \, dx$$

subject to

$$u \in W^{1,1}(0, 1), \qquad u(0) = u_0, \quad u(1) = u_1.$$

According to our discussion in the Introduction, the equivalent generalized variational principle in terms of Young measures associated to minimizing sequences takes the form [9]

$$\bar{I}(\nu) = \int_0^1 \int_{\mathbf{R}} \sum_{j=0}^{2n} a_j(x, u)\lambda^j \, d\nu_x(\lambda) \, dx,$$

where admissibility for $\nu = \{\nu_x\}_{x\in\Omega}$ means

$$\int_0^1 \int_{\mathbf{R}} |\lambda|^{2n} \, d\nu_x(\lambda) \, dx < \infty,$$

$$u'(x) = \int_{\mathbf{R}} \lambda \, d\nu_x(\lambda), \qquad u_1 - u_0 = \int_0^1 \int_{\mathbf{R}} \lambda \, d\nu_x(\lambda) \, dx.$$

The use of the Parseval identity is trivial in this situation and does not pose any technical difficulty since if we let

$$m_j(x) = \int_{\mathbf{R}} \lambda^j \, d\nu_x(\lambda),$$

the jth moment of ν_x, then we can write

$$\bar{I}(\nu) = \int_0^1 \sum_{j=0}^{2n} a_j(x, u) m_j(x) \, dx.$$

Looking at the vector $m = (m_j)_{j=0,1,\ldots,2n}$ as our independent variable, we can write $\bar{I}$ in terms of moments as

$$J(m) = \bar{I}(\nu) = \int_0^1 a(x, u(x)) \cdot m(x) \, dx,$$

$$a(x, u(x)) = (a_j(x, u(x)))_{j=0,1,\ldots,2n}, \qquad m = (m_j)_{j=0,1,\ldots,2n}.$$

Feasibility conditions on m will have to incorporate its genesis as succesive moments of probability measures, as well as the relationship between m and u, and prescribed boundary conditions. Namely,

$$m(x) \in \Lambda = \left\{ \left(\int_{\mathbf{R}} \lambda^i \, d\mu(\lambda) \right)_{i=0,1,\dots,2n} : \mu, \text{probability measure} \right\},$$
$$\text{for each} \quad x \in (0,1),$$
$$\int_0^1 m_1(x)\, dx = u_1 - u_0, \qquad u'(x) = m_1(x).$$

It is straightforward to check that Λ is a convex set of $\mathbf{R}^{2n+1}$. It is not closed due to the fact that in taking limits of a sequence of moments associated to a sequence of probability measures "some mass may escape to infinity." To clarify this issue consider the vector $(1, 0, 0, 0, 1)$ which belongs to the closure $\bar{\Lambda}$ because it is the limit of the vectors of moments up to fourth order of the sequence of probability measures

$$t\delta_{-((1-t)/t)^{1/4}} + (1-t)\delta_{(t/(1-t))^{1/4}},$$

when $t \to 1$. Indeed, the vector of moments corresponding to this sequence of measures is

$$(1, (t(1-t))^{1/4}(\sqrt{1-t} - \sqrt{t}), 2\sqrt{t(1-t)}, (t(1-t))^{1/4}(\sqrt{t} - \sqrt{1-t}), 1)$$

which converges to $(1, 0, 0, 0, 1)$ as $t \to 1$.

The whole point we would like to stress is that an independent characterization of the closure of the set Λ with no reference to any probability measure whatsoever exists. The key fact is the following theorem which is essentially a classical result on the algebraic moment problem [1], [10].

Theorem 2.1. *A vector $m = (m_j)_{j=0,1,2,\dots,2n}$, $m_0 = 1$, belongs to $\bar{\Lambda}$ if and only if its associated Hankel matrix*

$$H = (m_{k+l})_{k,l=0,1,\dots,n}, \qquad H = \begin{pmatrix} 1 & m_1 & m_2 & \cdots & m_n \\ m_1 & m_2 & m_3 & \cdots & m_{n+1} \\ m_2 & m_3 & & \cdots & m_{n+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_n & m_{n+1} & & \cdots & m_{2n} \end{pmatrix}$$

is positive semidefinite, i.e. all (real) eigenvalues are nonnegative.

Proof. Although as remarked earlier this is essentially a classical result, we include here some indication on how to deal with the closure of the set Λ. What is indeed classical is the following lemma.

Lemma 2.2 [1, page 30].

1. *If a vector* $m = (m_j)_{j=0,1,2,\ldots,2n}$, $m_0 = 1$, *belongs to* Λ, *then its associated Hankel matrix is positive semidefinite.*
2. *The Hankel matrix associated to a vector* m *as before is* (*strictly*) *positive definite if and only if* m *is the vector of the first* $2n$ *moments of a probability measure whose support contains at least* $n+1$ *different mass points.*

By an elementary perturbation argument based on this lemma we can prove our theorem.

The necessity part is straightforward from the lemma. Concerning the sufficiency, let m be such a vector whose Hankel matrix is positive semidefinite. Let μ be any probability measure supported in $\mathbf{R}$ whose vector of first $2n$ moments, $\tilde{m}$, gives rise to a positive definite Hankel matrix. For $\varepsilon > 0$ small, consider the vector

$$m^\varepsilon = \frac{1}{1+\varepsilon}(m + \varepsilon\tilde{m}),$$

and its associated Hankel matrix H_ε. By our assumption on m and the way in which we have chosen $\tilde{m}$, H_ε is positive definite. By Lemma 2.2 there exists a probability measure μ_ε whose vector of $2n$ first moments is m^ε. Hence $m^\varepsilon \in \Lambda$ and since $m^\varepsilon \to m$ as $\varepsilon \to 0$, we conclude that $m \in \bar{\Lambda}$ as desired. □

As a corollary we can express the condition on the eigenvalues of the matrix H in terms of its entries.

Corollary 2.3. *A vector* $m = (m_j)_{j=0,1,2,\ldots,2n}$, $m_0 = 1$, *belongs to* $\bar{\Lambda}$ *if and only if*

$$b_j \geq 0, \qquad j = 0, 1, 2, \ldots, n-1, n,$$

where b_j *are the coefficients of the characteristic polynomial of* H:

$$\det(H - \lambda\mathbf{1}) = \sum_{j=0}^{n+1} (-1)^j b_j \lambda^j.$$

The proof is based on the identification of $\bar{\Lambda}$ with the positive semidefinite Hankel matrices according to Theorem 2.1. A well-known result on the coefficients of the characteristic polynomial of a positive semidefinite matrix (e.g. [5] and [6]) completes the proof. However, since sometimes the characterization of symmetric, semidefinite matrices is formulated in different terms, we include here, for the convenience of the reader, some comments on the proof.

Proof of Corollary 2.3. Notice that the coefficients b_j are precisely $S_{n+1-j}(\lambda_0, \lambda_1, \ldots, \lambda_n)$ where S_d is the dth elementary symmetric function of the (real) eigenvalues of

H, λ_i. Therefore, it is well known that

$$\begin{aligned}\det(H - \lambda \mathbf{1}) &= (-1)^{n+1} \prod_{j=0}^{n} (\lambda - \lambda_j) \\ &= \sum_{j=0}^{n+1} (-1)^j S_{n+1-j}(\lambda_0, \lambda_1, \ldots, \lambda_n) \lambda^j \\ &= \sum_{j=0}^{n+1} (-1)^j b_j \lambda^j .\end{aligned}$$

If all eigenvalues λ_j are nonnegative, then trivially the coefficients b_j are also nonnegative. Conversely, if all b_j are nonnegative, then the characteristic polynomial written above cannot have a negative root $\lambda' < 0$ since, under the assumption $b_j \geq 0$ for all $j < n+1$, all terms in the above sum will have the same sign and its sum would vanish. This implies that each individual term

$$(-1)^j b_j \lambda'^j$$

must be zero. This in turn implies $b_j = 0$ for all $j < n + 1$. However, then the characteristic polynomial is $(-1)^{n+1}\lambda^{n+1}$ which obviously does not have a negative root. This contradiction finishes the proof. □

It is important to notice that, despite the fact that in the new variational problem in terms of the moments, we have to work on the closure of Λ because we have at our disposal such a characterization, the coercivity condition (1.1) (with $p = 2n$) forces optimal moment vectors to belong to Λ and not to $\bar{\Lambda} \backslash \Lambda$. In other words, the optimal solutions we are looking for must be the moments of the underlying Young measure solution, and these are truly probability measures whose mass is contained in a compact set of $\mathbf{R}$ and not a sequence of such probability measures for which part of the mass escapes to infinity. Even more, by Carathéodory's theorem [4] we know that the underlying Young measure solution is supported at most in two points, since we are working in one-dimensional problems. See [9] for a full discussion of this issue.

3. A Specific Example

We examine whether the results of the preceding section can lead to concrete conclusions in some cases. We concentrate on the case $n = 2$, so that we consider four-degree polynomials. In this section we show how this approach can be efficiently used to give the convexification of any four-degree polynomial in closed form in terms of its coefficients.

One of the simplest variational problems one can consider is

$$\text{Minimize} \quad \int_0^1 \varphi(u'(x))\, dx$$

subject to $u(0) = 0$, $u(1) = t$ and $u \in W^{1,1}(0, 1)$. It is well known that the value of this infimum is precisely the convexification of the scalar function $\varphi(s)$ evaluated at t, $C\varphi(t)$. Alternatively, we can also put

$$C\varphi(t) = \min\{\langle\varphi, \mu\rangle\colon\ \mu \text{ is a probability measure with first moment } t\}.$$

When φ is a polynomial of degree four, we can drop the linear part without loss of generality, and put

$$\varphi(s) = P(s) = a_2 s^2 + a_3 s^3 + s^4.$$

Due to the homogeneity of the situation, the above variational problem leading to the convexification of P at any given t is equivalent to

$$\min_m (a_2 m_2 + a_3 m_3 + m_4)$$

subject to the fact that (t, m_2, m_3, m_4) must be the moments of a probability measure. We now have at our disposal a fully explicit characterization of a vector $m = (m_1, m_2, m_3, m_4)$ to correspond to the moments of a probability measure, by direct application of Corollary 2.3.

Corollary 3.1. *A vector $m = (m_1, m_2, m_3, m_4)$ is the vector of the first four moments associated to a probability measure if and only if*

$$m_4 m_2 + m_4 + m_2 - m_1^2 - m_2^2 - m_3^2 \ge 0,$$
$$m_2 m_4 - m_3^2 - m_1^2 m_4 + 2m_1 m_2 m_3 - m_2^3 \ge 0.$$

Therefore, the problem of determining the convexification of P at t reduces to a convex, mathematical programming problem:

$$\min_m (a_2 m_2 + a_3 m_3 + m_4)$$

subject to

$$m_2 - t^2 + m_4 - m_2^2 + m_4 m_2 - m_3^2 \ge 0,$$
$$m_2 m_4 - m_3^2 - t^2 m_4 + 2t m_2 m_3 - m_2^3 \ge 0$$

Notice that in spite of the unboundedness of this set of vectors, the existence of an optimal solution is not an issue because we do know a priori that such an optimal solution must correspond to an optimal probability measure providing the convexification of our polynomial. It is this fully explicit problem we would like to treat. The Karush–Kuhn–Tucker optimality conditions read:

$$1 - \lambda_1(1 + m_2) - \lambda_2(m_2 - t^2) = 0,$$
$$a_3 - \lambda_1(-2m_3) - \lambda_2(-2m_3 + 2t m_2) = 0,$$

$$a_2 - \lambda_1(1 - 2m_2 + m_4) - \lambda_2(m_4 + 2tm_3 - 3m_2^2) = 0,$$
$$\lambda_1(m_2 - t^2 + m_4 - m_2^2 + m_4m_2 - m_3^2) = 0,$$
$$\lambda_2(m_2m_4 - m_3^2 - t^2m_4 + 2tm_2m_3 - m_2^3) = 0,$$
$$m_2 - t^2 + m_4 - m_2^2 + m_4m_2 - m_3^2 \geq 0,$$
$$m_2m_4 - m_3^2 - t^2m_4 + 2tm_2m_3 - m_2^3 \geq 0,$$
$$\lambda_1, \lambda_2 \geq 0,$$

where λ_1 and λ_2 are the multipliers associated to the two constraints. The case

$$\lambda_1 = \lambda_2 = 0$$

is clearly impossible. On the other hand the possibility

$$m_2 - t^2 + m_4 - m_2^2 + m_4m_2 - m_3^2 = 0,$$

together with the fact that the m_i's are the moments of a probability measure and therefore

$$m_2 - t^2 \geq 0, \qquad m_4 - m_2^2 \geq 0, \qquad m_4m_2 - m_3^2 \geq 0,$$

lead to the conclusion that the optimal underlying probability measure is a Dirac mass at t. This will correspond to the region where the polynomial is indeed convex. Finally, the region of nonconvexity must correspond to the case

$$\lambda_1 = 0, \qquad m_2 - t^2 + m_4 - m_2^2 + m_4m_2 - m_3^2 > 0,$$
$$m_2m_4 - m_3^2 - t^2m_4 + 2tm_2m_3 - m_2^3 = 0.$$

After eliminating λ_2 and appropriately rewriting the last equation, we arrive at the system of equations

$$(m_4 - m_2^2)(m_2 - t^2) - (tm_2 - m_3)^2 = 0,$$
$$a_3(m_2 - t^2) + 2(m_3 - tm_2) = 0,$$
$$a_2(m_2 - t^2) - m_4 - 2tm_3 + 3m_2^2 = 0.$$

By combining the last two, we get

$$m_4 - m_2 = (a_2 + ta_3 - 2m_2)(m_2 - t^2);$$

and by manipulating the first two, we have

$$m_4 - m_2^2 = \frac{a_3^2}{4}(m_2 - t^2).$$

We immediately see by looking at these two new equations that

$$m_2 = \frac{a_3^2}{8} - \frac{ta_3}{2} - \frac{a_2}{2},$$

and then

$$m_3 = \frac{a_2a_3}{4} - \frac{a_3^2}{16} + \left(\frac{3a_3^2}{8} - \frac{a_2}{2}\right)t,$$

$$m_4 = \frac{a_2^2}{4} - \frac{a_2a_3^2}{4} + \frac{3a_3^4}{64} + \left(\frac{a_2a_3}{2} - \frac{a_3^3}{4}\right)t.$$

These are the optimal moments when t does not belong to the convexity region of P. Altogether we can explicitly write down the straight line giving the linear part of CP, by taking these optimal moments and putting them in $a_2m_2 + a_3m_3 + m_4$ in order to obtain the affine expression in t:

$$\tfrac{1}{64}(-16a_2^2 + 8a_2a_3^2 - a_3^4) + \tfrac{1}{8}(-4a_2a_3 + a_3^3)t.$$

How can we determine the precise region where the convexification of P, CP, must coincide with P itself and where it must be the previous line? The common boundary of these two regimes can be determined by imposing that the optimal moments must be given simultaneously by the above formulas, and, at the same time, they must come from a single Dirac mass centered at t. Hence

$$\frac{a_3^2}{8} - \frac{ta_3}{2} - \frac{a_2}{2} = m_2 = t^2.$$

This quadratic equation yields the boundary values for t which separate the region where CP equals P and where it is equal to a straight line. Specifically,

$$CP(t) = \begin{cases} P(t), & |t + \frac{a_3}{4}| \geq \frac{1}{4}\sqrt{3a_3^2 - 8a_2}, \\ \frac{1}{64}(-16a_2^2 + 8a_2a_3^2 - a_3^4) & \\ \quad + \frac{1}{8}(-4a_2a_3 + a_3^3)t, & |t + \frac{a_3}{4}| \leq \frac{1}{4}\sqrt{3a_3^2 - 8a_2}. \end{cases} \tag{3.1}$$

When the radicand

$$3a_3^2 - 8a_2 \leq 0$$

the polynomial is indeed convex.

We believe it is worthwhile to compare this analysis to the more direct, geometric approach consisting of looking for points x and y such that

$$P'(x) = P'(y) = \frac{P(x) - P(y)}{x - y}.$$

The solution of these equations will also provide the necessary data for finding the convexification of P. However, the form of these equations when

$$P(s) = s^4 + a_3 s^3 + a_2 s^2$$

is

$$(x - y)[4(x^2 + xy + y^2) + 3a_3(x + y) + 2a_2] = 0,$$
$$(x^3 + x^2 y + xy^2 + y^3) + a_3(x^2 + xy + y^2) + a_2(x + y) = 4x^3 + 3a_3 x^2 + 2a_2 x.$$

This system of nonlinear equations does not seem as tractable as the one we have solved before. In fact, we had to resort to a symbolic calculator package in order to find the solution in closed form.

Needless to say, it is impossible to provide the fully explicit form of the convexification for a general sixth- or higher-degree polynomial in terms of the coefficients as in (3.1), although the procedure works reasonably well for concrete, specific examples.

We believe it is also interesting to stress the point that if we use the fact that optimal vector of moments must correspond to convex combinations of just two Dirac masses (as pointed out before) too soon, then the good convexity properties of our formulation are lost and, despite the fact that the number of variables may be considerably reduced, one has to deal with local minima. Again, the main feature of the moment formulation is that it definitely avoids the difficulties attached to local minima.

4. Numerical Computations

From our perspective, the most interesting feature of the analysis proposed in this paper is that the new formulation in terms of moments corresponds to minimizing a linear cost functional under a set of constraints determining a convex set of feasible vectors. This is again what the title of the paper means to convey. From the numerical approximation viewpoint, this is a quite remarkable transformation since the new formulation is suitable for the use of standard optimization algorithms. In particular, it completely avoids the tremendous difficulty attached to local minima. We would like to stress this point by looking at a number of selected examples and conducting several numerical experiments on them. Some attempts to compute the underlying Young measure for some of these same examples have been made in [3] and [8].

We remind the reader that the type of problem we are concerned with is

$$\text{Minimize} \quad \int_0^1 \sum_{j=0}^{2n} a_j(x, u(x)) u'(x)^j \, dx$$

subject to

$$u \in W^{1,1}(0, 1), \qquad u(0) = u_0, \quad u(1) = u_1.$$

Although in principle the procedure would work for any n, for simplicity we restrict attention to $n = 2$, so that we are again dealing with fourth-degree polynomials in the derivative u'.

The equivalent, linear, convex, fully explicit optimization problem would read

$$\text{Minimize} \quad \int_0^1 \sum_{j=0}^{4} a_j(x, u(x)) m_j(x)\, dx$$

subject to

$$m_4(x)m_2(x) + m_4(x) + m_2(x) - m_1(x)^2 - m_2(x)^2 - m_3(x)^2 \geq 0,$$
$$m_2(x)m_4(x) - m_3(x)^2 - m_1(x)^2 m_4(x) + 2m_1(x)m_2(x)m_3(x) - m_2(x)^3 \geq 0,$$
$$u'(x) = m_1(x), \qquad \int_0^1 m_1(x)\, dx = u_1 - u_0.$$

We adopt a typical discretization based on equally spaced nodes in the interval (0, 1). All of our experiments were conducted by dividing this interval into 10 subintervals. Discrete moments are assumed to be constant on each subinterval where we utilize a usual trapezoidal rule to integrate numerically the coefficients $a_j(x, u(x))$ on a given subinterval. The form of the discretized version is

$$\text{Minimize} \quad \frac{1}{20} \sum_{i=1}^{10} \sum_{j=0}^{4} \left[a_j \left(\frac{i}{10}, u_0 + \frac{1}{10} \sum_{k=1}^{i} m_1^{(k)} \right) + a_j \left(\frac{i-1}{10}, u_0 + \frac{1}{10} \sum_{k=1}^{i-1} m_1^{(k)} \right) \right] m_j^{(i)}$$

subject to

$$m_4^{(i)} m_2^{(i)} + m_4^{(i)} + m_2^{(i)} - (m_1^{(i)})^2 - (m_2^{(i)})^2 - (m_3^{(i)})^2 \geq 0, \qquad i = 1, 2, \ldots, 10,$$
$$m_2^{(i)} m_4^{(i)} - (m_3^{(i)})^2 - (m_1^{(i)})^2 m_4^{(i)} + 2m_1^{(i)} m_2^{(i)} m_3^{(i)} - (m_2^{(i)})^3 \geq 0, \qquad i = 1, 2, \ldots, 10,$$
$$\frac{1}{10} \sum_{i=1}^{10} m_1^{(i)} = u_1 - u_0.$$

The variables of the problem are the discretized moments

$$\{m_j^{(i)}\}_{i=1,2,\ldots,10,\, j=0,1,\ldots,4}.$$

Notice that if the dependence of the coefficients a_j is nonlinear on u, a nonlinearity is introduced on the cost functional when eliminating u from the formulation. This dependence needs to be convex. It is this discretized version that can be approximated by standard optimization algorithms or packages. Notice that we are dealing with a convex problem so that numerical algorithms should provide the global minimum.

Once this optimal solution $\{m_j^{(i)}\}$ is found, we need to recover the underlying probability measures

$$\nu^{(i)} = w^{(i)}\delta_{l^{(i)}} + (1 - w^{(i)})\delta_{r^{(i)}}, \qquad i = 1, 2, \ldots, 10,$$

whose moments up to fourth order are precisely the optimal solution found. This is an easy elementary task. Since we are in the one-dimensional situation, one weight

$$w^{(i)} \in [0, 1]$$

and two mass points

$$l^{(i)} \le r^{(i)}$$

suffice. These three parameters are the solution of the system

$$\begin{aligned}
&w^{(i)}l^{(i)} + (1 - w^{(i)})r^{(i)} = m_1^{(i)},\\
&w^{(i)}(l^{(i)})^2 + (1 - w^{(i)})(r^{(i)})^2 = m_2^{(i)},\\
&w^{(i)}(l^{(i)})^3 + (1 - w^{(i)})(r^{(i)})^3 = m_3^{(i)},
\end{aligned}$$

for each i. Explicit formulae for the solution can be given.

This family of probability measures can be interpreted as a discretized version of the underlying Young measure minimizer of the original nonconvex variational problem (see [9]). The way in which we can depict minimizing sequences from those probability measures consists in drawing on each subinterval $(i - \frac{1}{10}, i/10)$ small line segments with relative length given by the weight $w^{(i)}$ and alternate slopes $l^{(i)}$ and $r^{(i)}$. Optimal behavior would tend to refine indefinitely these small segments. From this point of view, it is important to realize that our computations are not finite-element approximations. In the numerical table that follows, we provide those weights, $w^{(i)}$ and $1 - w^{(i)}$, associated with mass points $r^{(i)}$ and $l^{(i)}$, respectively. By using this information as we have just explained, pictures of minimizing sequences are drawn.

The numerical algorithm we have used consists of a quadratic penalization to take care of the nonnegative constraints. The optimization algorithm itself is a typical conjugate gradient method. More accurate approximations would require a much more specialized analysis. Yet our results faithfully reflect the behavior of minimizing sequences.

We have first computed several examples where the optimal, oscillatory behavior is known, at least qualitatively. Then we explore more complex examples where nothing is known about optimality.

We first take the typical two-well potential where the functional is given by

$$I(u) = \int_0^1 [(u'(x)^2 - 1)^2 + \tfrac{1}{2}u(x)^2]\,dx.$$

Numerical results for this functional depending on boundary conditions are given in Table 1.

Table 1. Numerical results for different boundary conditions.

	Weight	Slope	Weight	Slope
	Boundary conditions: $u_0 = u_1 = 0$			
$n = 1$	0.496516	0.988789	0.503484	−0.984965
$n = 2$	0.496496	0.988778	0.503504	−0.985006
$n = 3$	0.496702	0.988531	0.503298	−0.985131
$n = 4$	0.496298	0.988674	0.503702	−0.985388
$n = 5$	0.496985	0.988067	0.503015	−0.985475
$n = 6$	0.497278	0.987665	0.502722	−0.985724
$n = 7$	0.497548	0.987257	0.502452	−0.985998
$n = 8$	0.497893	0.986760	0.502107	−0.986317
$n = 9$	0.498285	0.986199	0.501715	−0.986663
$n = 10$	0.498755	0.985552	0.501245	−0.987055
	Boundary conditions: $u_0 = 0$, $u_1 = \frac{1}{2}$			
$n = 1$	0.713578	0.873943	0.286422	−0.961861
$n = 2$	0.725119	0.876012	0.274881	−0.972898
$n = 3$	0.742838	0.879419	0.257162	−0.992038
$n = 4$	0.762479	0.883814	0.237521	−1.01651
$n = 5$	0.783088	0.888899	0.216912	−1.04602
$n = 6$	0.804777	0.894646	0.195223	−1.08274
$n = 7$	0.827228	0.901196	0.172772	−1.12872
$n = 8$	0.850084	0.908649	0.149916	−1.18569
$n = 9$	0.873063	0.917012	0.126937	−1.25862
$n = 10$	0.895716	0.926377	0.104284	−1.35229

These results reflect what was already known. In the first case the Young measure solution is homogeneous, essentially the same in all subintervals. This is not so however for the other set of boundary conditions. If we draw these numerical values, the profile of the solutions for each of the above situations would be the ones shown in Figures 1 and 2.

Our next example consists of an interesting variation of the preceding one where we change the zero-degree contribution of the functional, namely,

$$I(u) = \int_0^1 \left[(u'(x)^2 - 1)^2 + \frac{1}{2}\left(u(x) - \frac{x}{2} \right)^2 \right] dx.$$

This particular case, and the effect of boundary conditions on the Young measure solution was thoroughly examined in [7]. Our numerical results agree with the conclusions on this reference. Notice how in some cases there is a region where the Young measure solution is trivial so that optimal behavior will not exhibit oscillations in that zone. Rather than giving the numerical values obtained in this and subsequent examples we have depicted them in a graph (Figures 3–5).

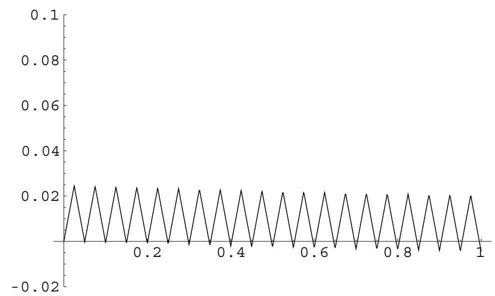

Figure 1. Boundary conditions: $u_0 = u_1 = 0$.

Our next example was also considered in [7]. This time the functional and boundary conditions are

$$I(u) = \int_0^1 [(u'(x)^2 - 1)^2 + \tfrac{1}{2}(u(x) - 2x(x-1))^2]\,dx, \qquad u(0) = u(1) = 0.$$

The second draft in Figures 6 and 7 are a magnified version of the central part of the interval where persistent oscillations occur.

Our final example is the functional

$$I(u) = \int_0^1 [u'(x)^4 + u(x)u'(x)^3 + (u(x) - x)^2]\,dx.$$

We used two sets of boundary conditions. In the first instance, we put $u_0 = 0$, $u_1 = 0.3$. The computed optimal behavior we found is shown in Figures 8 and 9. Secondly, we took $u_0 = 0$, $u_1 = -0.3$, and obtained the profiles given in Figures 10 and 11.

In subsequent papers we would like to analyze whether these ideas can be implemented in the (scalar) higher-dimensional situation.

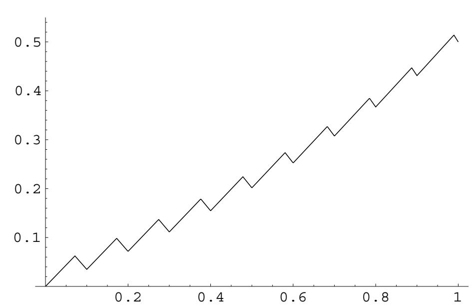

Figure 2. Boundary conditions: $u_0 = 0$, $u_1 = \frac{1}{2}$.

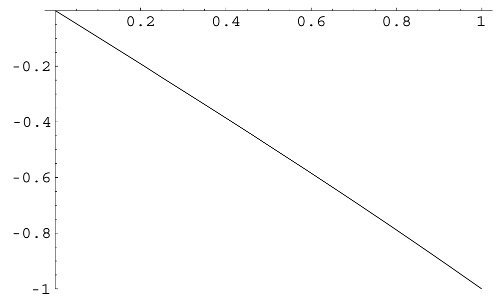

Figure 3. Boundary conditions: $u_0 = 0$, $u_1 = -1$.

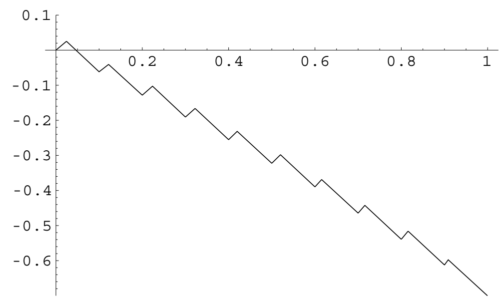

Figure 4. Boundary conditions: $u_0 = 0$, $u_1 = -0.7$.

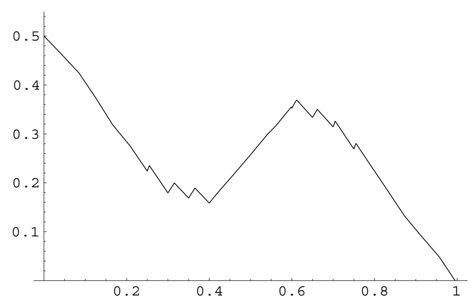

Figure 5. Boundary conditions: $u_0 = 0.5$, $u_1 = 0$.

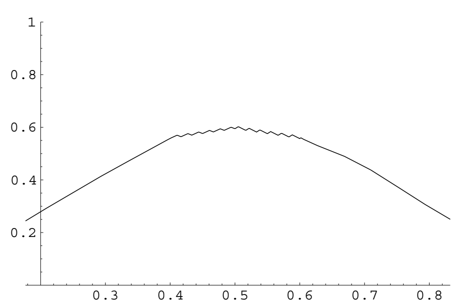

Figure 6.

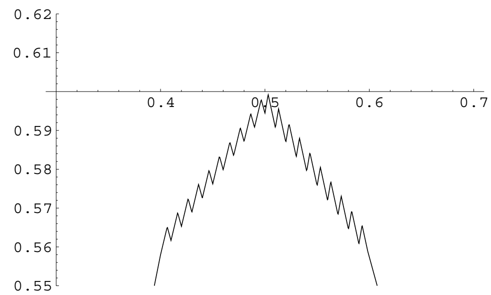

Figure 7.

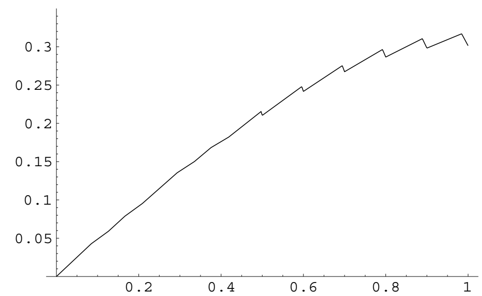

Figure 8.

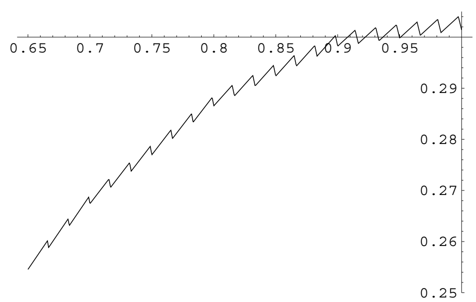

Figure 9.

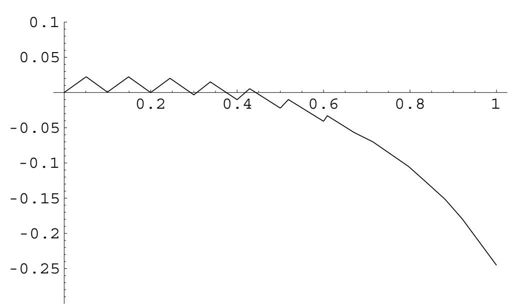

Figure 10.

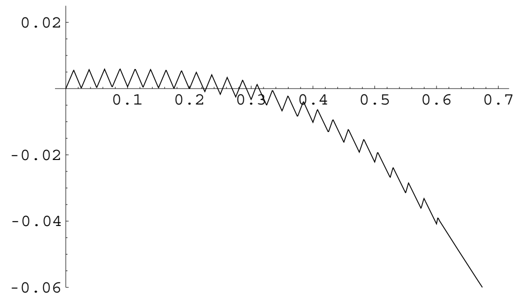

Figure 11.

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