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Keywords: Duality theory; non-convex analysis; numerical method for a non-smooth model



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Article

# Duality Principles and Numerical Procedures for a Large Class of Non-Convex Models in the Calculus of Variations

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**Abstract:** This article develops duality principles and numerical results for a large class of non-convex variational models. The main results are based on fundamental tools of convex analysis, duality theory and calculus of variations. More specifically the approach is established for a class of non-convex functionals similar as those found in some models in phase transition. Finally, in the last section we present a concerning numerical example and the respective software.

**Keywords:** duality theory; non-convex analysis; numerical method for a non-smooth model

**MSC:** 49N15

## 1. Introduction

In this section we establish a dual formulation for a large class of models in non-convex optimization.

The main duality principle is applied to double well models similar as those found in the phase transition theory.

Such results are based on the works of J.J. Telega and W.R. Bielski [2,3,13,14] and on a D.C. optimization approach developed in Toland [15].

About the other references, details on the Sobolev spaces involved are found in [1]. Related results on convex analysis and duality theory are addressed in [5–7,9,12].

Finally, in this text we adopt the standard Einstein convention of summing up repeated indices, unless otherwise indicated.

In order to clarify the notation, here we introduce the definition of topological dual space.

**Definition 1.1** (Topological dual spaces). *Let  $U$  be a Banach space. We shall define its dual topological space, as the set of all linear continuous functionals defined on  $U$ . We suppose such a dual space of  $U$ , may be represented by another Banach space  $U^*$ , through a bilinear form  $\langle \cdot, \cdot \rangle_U : U \times U^* \rightarrow \mathbb{R}$  (here we are referring to standard representations of dual spaces of Sobolev and Lebesgue spaces). Thus, given  $f : U \rightarrow \mathbb{R}$  linear and continuous, we assume the existence of a unique  $u^* \in U^*$  such that*

$$f(u) = \langle u, u^* \rangle_U, \forall u \in U. \quad (1)$$

The norm of  $f$ , denoted by  $\|f\|_{U^*}$ , is defined as

$$\|f\|_{U^*} = \sup_{u \in U} \{ |\langle u, u^* \rangle_U| : \|u\|_U \leq 1 \} \equiv \|u^*\|_{U^*}. \quad (2)$$

At this point we start to describe the primal and dual variational formulations.

## 2. A general duality principle non-convex optimization

In this section we present a duality principle applicable to a model in phase transition.

This case corresponds to the vectorial one in the calculus of variations.

Let  $\Omega \subset \mathbb{R}^n$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

Consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = F(\nabla u_1, \dots, \nabla u_N) + G(u_1, \dots, u_N) - \langle u_i, f_i \rangle_{L^2},$$

and where

$$V = \{u = (u_1, \dots, u_N) \in W^{1,p}(\Omega; \mathbb{R}^N) : u = u_0 \text{ on } \partial\Omega\},$$

$f \in L^2(\Omega; \mathbb{R}^N)$ , and  $1 < p < +\infty$ .

We assume there exists  $\alpha \in \mathbb{R}$  such that

$$\alpha = \inf_{u \in V} J(u).$$

Moreover, suppose  $F$  and  $G$  are Fréchet differentiable but not necessarily convex. A global optimum point may not be attained for  $J$  so that the problem of finding a global minimum for  $J$  may not be a solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of  $J$ .

We intend to use duality theory to approximately solve such a global optimization problem.

Denoting  $V_0 = W_0^{1,p}(\Omega; \mathbb{R}^N)$ ,  $Y_1 = Y_1^* = L^2(\Omega; \mathbb{R}^{N \times n})$ ,  $Y_2 = Y_2^* = L^2(\Omega; \mathbb{R}^{N \times n})$ ,  $Y_3 = Y_3^* = L^2(\Omega; \mathbb{R}^N)$ , at this point we define,  $F_1 : V \times V_0 \rightarrow \mathbb{R}$ ,  $G_1 : V \rightarrow \mathbb{R}$ ,  $G_2 : V \rightarrow \mathbb{R}$ ,  $G_3 : V_0 \rightarrow \mathbb{R}$  and  $G_4 : V \rightarrow \mathbb{R}$ , by

$$\begin{aligned} F_1(\nabla u, \nabla \phi) &= F(\nabla u_1 + \nabla \phi_1, \dots, \nabla u_N + \nabla \phi_N) + \frac{K}{2} \int_{\Omega} \nabla u_j \cdot \nabla u_j \, dx \\ &\quad + \frac{K_2}{2} \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_j \, dx \end{aligned} \quad (3)$$

and

$$G_1(u_1, \dots, u_n) = G(u_1, \dots, u_N) + \frac{K_1}{2} \int_{\Omega} u_j u_j \, dx - \langle u_i, f_i \rangle_{L^2},$$

$$G_2(\nabla u_1, \dots, \nabla u_N) = \frac{K_1}{2} \int_{\Omega} \nabla u_j \cdot \nabla u_j \, dx,$$

$$G_3(\nabla \phi_1, \dots, \nabla \phi_N) = \frac{K_2}{2} \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_j \, dx,$$

and

$$G_4(u_1, \dots, u_N) = \frac{K_1}{2} \int_{\Omega} u_j u_j \, dx.$$

Define now  $J_1 : V \times V_0 \rightarrow \mathbb{R}$ ,

$$J_1(u, \phi) = F(\nabla u + \nabla \phi) + G(u) - \langle u_i, f_i \rangle_{L^2}.$$

Observe that

$$\begin{aligned}
J_1(u, \phi) &= F_1(\nabla u, \nabla \phi) + G_1(u) - G_2(\nabla u) - G_3(\nabla \phi) - G_4(u) \\
&\leq F_1(\nabla u, \nabla \phi) + G_1(u) - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\
&\quad + \sup_{v_1 \in Y_1} \{ \langle v_1, z_1^* \rangle_{L^2} - G_2(v_1) \} \\
&\quad + \sup_{v_2 \in Y_2} \{ \langle v_2, z_2^* \rangle_{L^2} - G_3(v_2) \} \\
&\quad + \sup_{u \in V} \{ \langle u, z_3^* \rangle_{L^2} - G_4(u) \} \\
&= F_1(\nabla u, \nabla \phi) + G_1(u) - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*) \\
&= J_1^*(u, \phi, z^*),
\end{aligned} \tag{4}$$

$\forall u \in V, \phi \in V_0, z^* = (z_1^*, z_2^*, z_3^*) \in Y^* = Y_1^* \times Y_2^* \times Y_3^*$ .

Here we assume  $K, K_1, K_2$  are large enough so that  $F_1$  and  $G_1$  are convex.

Hence, from the general results in [15], we may infer that

$$\inf_{(u, \phi) \in V \times V_0} J(u, \phi) = \inf_{(u, \phi, z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*). \tag{5}$$

On the other hand

$$\inf_{u \in V} J(u) \geq \inf_{(u, \phi) \in V \times V_0} J_1(u, \phi) \geq \inf_{u \in V} Q_J(u) = \inf_{u \in V} J(u),$$

where  $Q_J(u)$  refers to a standard quasi-convex regularization of  $J$ .

From these last two results we may obtain

$$\inf_{u \in V} J(u) = \inf_{(u, \phi, z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*).$$

Moreover, from standards results on convex analysis, we may have

$$\begin{aligned}
\inf_{u \in V} J_1^*(u, \phi, z^*) &= \inf_{u \in V} \{ F_1(\nabla u, \nabla \phi) + G_1(u) \\
&\quad - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*) \} \\
&= \sup_{(v_1^*, v_2^*) \in C^*} \{ -F_1^*(v_1^* + z_1^*, \nabla \phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla \phi, z_2^* \rangle_{L^2} \\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*) \},
\end{aligned} \tag{6}$$

where

$$C^* = \{ v^* = (v_1^*, v_2^*) \in Y_1^* \times Y_3^* : -\operatorname{div}(v_1^*)_i + (v_2^*)_i = 0, \forall i \in \{1, \dots, N\} \},$$

$$F_1^*(v_1^* + z_1^*, \nabla \phi) = \sup_{v_1 \in Y_1} \{ \langle v_1, z_1^* + v_1^* \rangle_{L^2} - F_1(v_1, \nabla \phi) \},$$

and

$$G_1^*(v_2^* + z_3^*) = \sup_{u \in V} \{ \langle u, v_2^* + z_3^* \rangle_{L^2} - G_1(u) \}.$$

Thus, defining

$$J_2^*(\phi, z^*, v^*) = F_1^*(v_1^* + z_1^*, \nabla \phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla \phi, z_2^* \rangle_{L^2} + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*),$$

we have got

$$\begin{aligned}
 \inf_{u \in V} J(u) &= \inf_{(u, \phi) \in V \times V_0} J_1(u, \phi) \\
 &= \inf_{(u, \phi, z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*) \\
 &= \inf_{z^* \in Y^*} \left\{ \inf_{\phi \in V_0} \left\{ \sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*) \right\} \right\}. \tag{7}
 \end{aligned}$$

Finally, observe that

$$\begin{aligned}
 \inf_{u \in V} J(u) &= \inf_{z^* \in Y^*} \left\{ \inf_{\phi \in V_0} \left\{ \sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*) \right\} \right\} \\
 &\geq \sup_{v^* \in C^*} \left\{ \inf_{(z^*, \phi) \in Y^* \times V_0} J_2^*(\phi, z^*, v^*) \right\}. \tag{8}
 \end{aligned}$$

This last variational formulation corresponds to a concave relaxed formulation in  $v^*$  concerning the original primal formulation.

### 3. Another duality principle for a simpler related model in phase transition with a respective numerical example

In this section we present another duality principle for a related model in phase transition.

Let  $\Omega = [0, 1] \subset \mathbb{R}$  and consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{1}{2} \int_{\Omega} ((u')^2 - 1)^2 dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and where

$$V = \{u \in W^{1,4}(\Omega) : u(0) = 0 \text{ and } u(1) = 1/2\}$$

and  $f \in L^2(\Omega)$ .

A global optimum point is not attained for  $J$  so that the problem of finding a global minimum for  $J$  has no solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of  $J$ .

We intend to use duality theory to approximately solve such a global optimization problem.

Denoting  $V_0 = W_0^{1,4}(\Omega)$ , at this point we define,  $F : V \rightarrow \mathbb{R}$  and  $F_1 : V \times V_0 \rightarrow \mathbb{R}$  by

$$F(u) = \frac{1}{2} \int_{\Omega} ((u')^2 - 1)^2 dx,$$

and

$$F_1(u, \phi) = \frac{1}{2} \int_{\Omega} ((u' + \phi')^2 - 1)^2 dx.$$

Observe

$$F(u) \geq \inf_{\phi \in V_0} F_1(u, \phi) \geq Q_F(u), \quad \forall u \in V,$$

where  $Q_F(u)$  refers to a quasi-convex regularization of  $F$ .

We define also

$$F_2 : V \times V_0 \rightarrow \mathbb{R},$$

$$F_3 : V \times V_0 \rightarrow \mathbb{R}$$

and

$$G : V \times V_0 \rightarrow \mathbb{R}$$

by

$$\begin{aligned} F_2(u, \phi) &= \frac{1}{2} \int_{\Omega} ((u' + \phi')^2 - 1)^2 dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2}, \\ F_3(u, \phi) &= F_2(u, \phi) + \frac{K}{2} \int_{\Omega} (u')^2 dx \\ &\quad + \frac{K_1}{2} \int_{\Omega} (\phi')^2 dx \end{aligned} \quad (9)$$

and

$$\begin{aligned} G(u, \phi) &= \frac{K}{2} \int_{\Omega} (u')^2 dx \\ &\quad + \frac{K_1}{2} \int_{\Omega} (\phi')^2 dx \end{aligned} \quad (10)$$

Observe that if  $K > 0, K_1 > 0$  is large enough, both  $F_3$  and  $G$  are convex.

Denoting  $Y = Y^* = L^2(\Omega)$  we also define the polar functional  $G^* : Y^* \times Y^* \rightarrow \mathbb{R}$  by

$$G^*(v^*, v_0^*) = \sup_{(u, \phi) \in V \times V_0} \{ \langle u, v^* \rangle_{L^2} + \langle \phi, v_0^* \rangle_{L^2} - G(u, \phi) \}.$$

Observe that

$$\inf_{u \in U} J(u) \geq \inf_{((u, \phi), (v^*, v_0^*)) \in V \times V_0 \times [Y^*]^2} \{ G^*(v^*, v_0^*) - \langle u, v^* \rangle_{L^2} - \langle \phi, v_0^* \rangle_{L^2} + F_3(u, \phi) \}.$$

With such results in mind, we define a relaxed primal dual variational formulation for the primal problem, represented by  $J_1^* : V \times V_0 \times [Y^*]^2 \rightarrow \mathbb{R}$ , where

$$J_1^*(u, \phi, v^*, v_0^*) = G^*(v^*, v_0^*) - \langle u, v^* \rangle_{L^2} - \langle \phi, v_0^* \rangle_{L^2} + F_3(u, \phi).$$

Having defined such a functional, we may obtain numerical results by solving a sequence of convex auxiliary sub-problems, through the following algorithm.

1. Set  $K \approx 150$  and  $K_1 = K/20$  and  $0 < \varepsilon \ll 1$ .
2. Choose  $(u_1, \phi_1) \in V \times V_0$ , such that  $\|u_1\|_{1, \infty} \ll K/4$  and  $\|\phi_1\|_{1, \infty} \ll K/4$ .
3. Set  $n = 1$ .
4. Calculate  $(v_n^*, (v_0^*)_n)$  solution of the system of equations:

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v^*} = \mathbf{0}$$

and

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v_0^*} = \mathbf{0},$$

that is

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v^*} - u_n = 0$$

and

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v_0^*} - \phi_n = 0$$

so that

$$v_n^* = \frac{\partial G(u_n, \phi_n)}{\partial u}$$

and

$$(v_0^*)_n = \frac{\partial G(u_n, \phi_n)}{\partial \phi}$$

5. Calculate  $(u_{n+1}, \phi_{n+1})$  by solving the system of equations:

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial u} = \mathbf{0}$$

and

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial \phi} = \mathbf{0}$$

that is

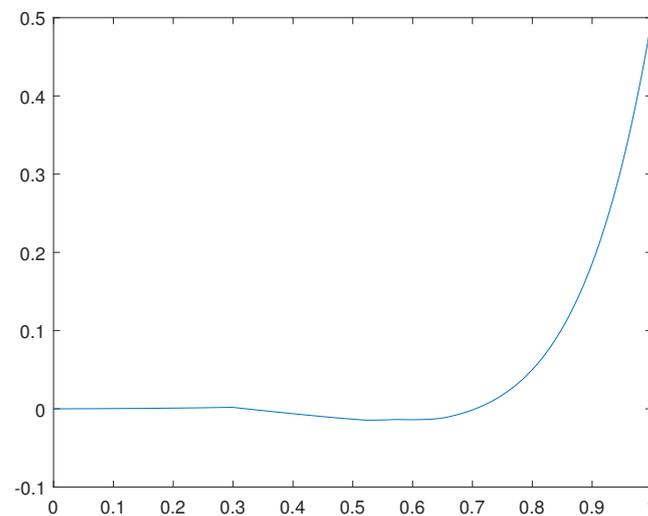
$$-v_n^* + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial u} = \mathbf{0}$$

and

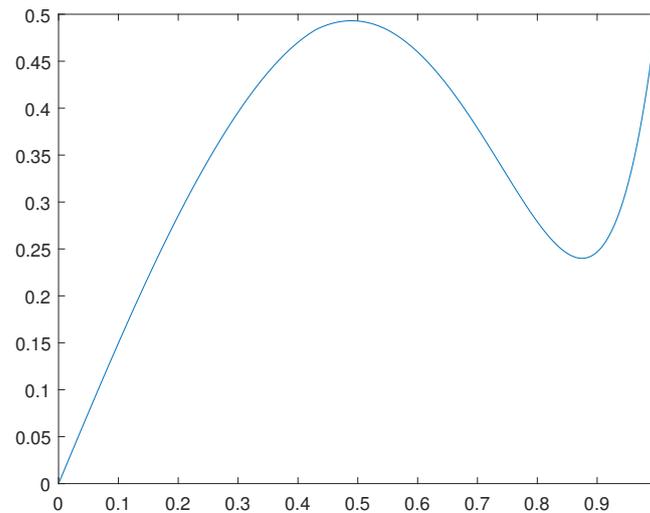
$$-(v_0^*)_n + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial \phi} = \mathbf{0}$$

6. If  $\max\{\|u_n - u_{n+1}\|_\infty, \|\phi_{n+1} - \phi_n\|_\infty\} \leq \varepsilon$ , then stop, else set  $n := n + 1$  and go to item 4.

For the case in which  $f(x) = 0$ , we have obtained numerical results for  $K = 1500$  and  $K_1 = K/20$ . For such a concerning solution  $u_0$  obtained, please see Figure 1. For the case in which  $f(x) = \sin(\pi x)/2$ , we have obtained numerical results for  $K = 100$  and  $K_1 = K/20$ . For such a concerning solution  $u_0$  obtained, please see Figure 2.



**Figure 1.** solution  $u_0(x)$  for the case  $f(x) = 0$ .



**Figure 2.** solution  $u_0(x)$  for the case  $f(x) = \sin(\pi x)/2$ .

**Remark 3.1.** Observe that the solutions obtained are approximate critical points. They are not, in a classical sense, the global solutions for the related optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.

#### 4. A convex dual variational formulation for a third similar model

In this section we present another duality principle for a third related model in phase transition. Let  $\Omega = [0, 1] \subset \mathbb{R}$  and consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{1}{2} \int_{\Omega} \min\{(u' - 1)^2, (u' + 1)^2\} dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and where

$$V = \{u \in W^{1,2}(\Omega) : u(0) = 0 \text{ and } u(1) = 1/2\}$$

and  $f \in L^2(\Omega)$ .

A global optimum point is not attained for  $J$  so that the problem of finding a global minimum for  $J$  has no solution.

Anyway, one question remains, how the minimizing sequences behave close to the infimum of  $J$ .

We intend to use the duality theory to solve such a global optimization problem in an appropriate sense to be specified.

At this point we define,  $F : V \rightarrow \mathbb{R}$  and  $G : V \rightarrow \mathbb{R}$  by

$$\begin{aligned} F(u) &= \frac{1}{2} \int_{\Omega} \min\{(u' - 1)^2, (u' + 1)^2\} dx \\ &= \frac{1}{2} \int_{\Omega} (u')^2 dx - \int_{\Omega} |u'| dx + 1/2 \\ &\equiv F_1(u'), \end{aligned} \tag{11}$$

and

$$G(u) = \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2}.$$

Denoting  $Y = Y^* = L^2(\Omega)$  we also define the polar functional  $F_1^* : Y^* \rightarrow \mathbb{R}$  and  $G^* : Y^* \rightarrow \mathbb{R}$  by

$$\begin{aligned}
 F_1^*(v^*) &= \sup_{v \in Y} \{ \langle v, v^* \rangle_{L^2} - F_1(v) \} \\
 &= \frac{1}{2} \int_{\Omega} (v^*)^2 dx + \int_{\Omega} |v^*| dx,
 \end{aligned} \tag{12}$$

and

$$\begin{aligned}
 G^*((v^*)') &= \sup_{u \in V} \{ -\langle u', v^* \rangle_{L^2} - G(u) \} \\
 &= \frac{1}{2} \int_{\Omega} ((v^*)' + f)^2 dx - \frac{1}{2} v^*(1).
 \end{aligned} \tag{13}$$

Observe this is the scalar case of the calculus of variations, so that from the standard results on convex analysis, we have

$$\inf_{u \in V} J(u) = \max_{v^* \in Y^*} \{ -F_1^*(v^*) - G^*(-(v^*)') \}.$$

Indeed, from the direct method of the calculus of variations, the maximum for the dual formulation is attained at some  $\hat{v}^* \in Y^*$ .

Moreover, the corresponding solution  $u_0 \in V$  is obtained from the equation

$$u_0 = \frac{\partial G((\hat{v}^*)')}{\partial (\hat{v}^*)'} = (\hat{v}^*)' + f.$$

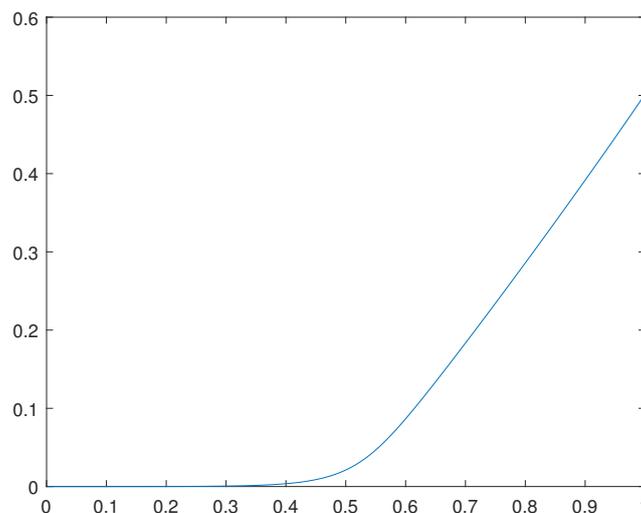
Finally, the Euler-Lagrange equations for the dual problem stands for

$$\begin{cases} (\hat{v}^*)'' + f' - \hat{v}^* - \text{sign}(\hat{v}^*) = 0, & \text{in } \Omega, \\ (\hat{v}^*)'(0) = 0, (\hat{v}^*)'(1) = 1/2. \end{cases} \tag{14}$$

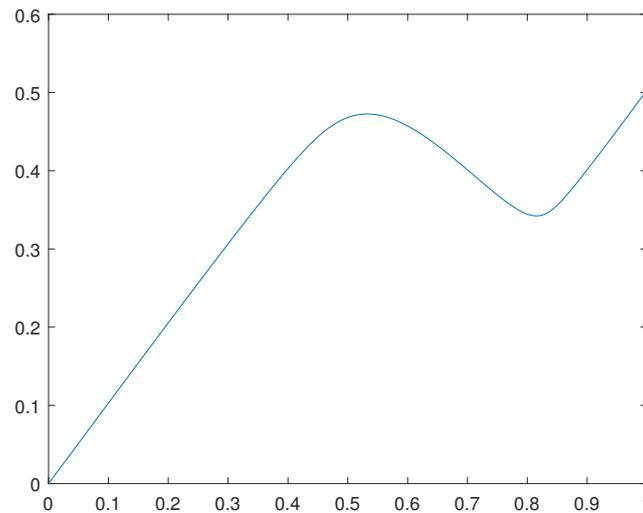
We have computed the solutions  $v^*$  and corresponding solutions  $u_0 \in V$  for the cases in which  $f(x) = 0$  and  $f(x) = \sin(\pi x)/2$ .

For the solution  $u_0(x)$  for the case in which  $f(x) = 0$ , please see Figure 3.

For the solution  $u_0(x)$  for the case in which  $f(x) = \sin(\pi x)/2$ , please see Figure 4.



**Figure 3.** solution  $u_0(x)$  for the case  $f(x) = 0$ .



**Figure 4.** solution  $u_0(x)$  for the case  $f(x) = \sin(\pi x)/2$ .

**Remark 4.1.** Observe that such solutions  $u_0$  obtained are not the global solutions for the related primal optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.

#### 4.1. The algorithm through which we have obtained the numerical results

In this subsection we present the software in MATLAB through which we have obtained the last numerical results.

This algorithm is for solving the concerning Euler-Lagrange equations for the dual problem, that is, for solving the equation

$$\begin{cases} (v^*)'' + f' - v^* - \text{sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) = 0, (v^*)'(1) = 1/2. \end{cases} \quad (15)$$

Here the concerning software in MATLAB. We emphasize to have used the smooth approximation

$$|v^*| \approx \sqrt{(v^*)^2 + e_1},$$

where a small value for  $e_1$  is specified in the next lines.

```
*****
1. clear all
2. m8 = 800; (number of nodes)
3. d = 1/m8;
4. e1 = 0.00001;
5. for i = 1 : m8
    yo(i,1) = 0.01;
    y1(i,1) = sin(pi * i/m8)/2;
end;
6. for i = 1 : m8 - 1
    dy1(i,1) = (y1(i + 1,1) - y1(i,1))/d;
end;
```

```

7. for k = 1 : 3000 (we have fixed the number of iterations)
    i = 1;
    h3 = 1/√(v0(i,1)² + e1);
    m12 = 1 + d² * h3 + d²;
    m50(i) = 1/m12;
    z(i) = m50(i) * (dy1(i,1) * d²);
8. for i = 2 : m8 - 1
    h3 = 1/√(v0(i,1)² + e1);
    m12 = 2 + h3 * d² + d² - m50(i - 1);
    m50(i) = 1/m12;
    z(i) = m50(i) * (z(i - 1) + dy1(i,1) * d²);
    end;
9. v(m8, 1) = (d/2 + z(m8 - 1))/(1 - m50(m8 - 1));
10. for i = 1 : m8 - 1
    v(m8 - i, 1) = m50(m8 - i) * v(m8 - i + 1) + z(m8 - i);
    end;
11. v(m8/2, 1)
12. v0 = v;
    end;
13. for i = 1 : m8 - 1
    u(i, 1) = (v(i + 1, 1) - v(i, 1))/d + y1(i, 1);
    end;
14. for i = 1 : m8 - 1
    x(i) = i * d;
    end;
    plot(x, u(:, 1))

```

\*\*\*\*\*

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