A FIRST STEP TOWARDS VARIATIONAL METHODS IN ENGINEERING

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Abstract. In this paper, a didactical proposal to introduce the variational methods for solving boundary value problems to engineering students is presented. Starting from a couple of simple models arising in linear elasticity and heat diffusion, it is motivated the concept of weak solution for those models and it is proved the existence, uniqueness and continuous dependence on the initial data for these solutions. Finally, the solutions of the above mentioned problems are numerically evaluated by the finite element method.

1. Introduction

The importance of mathematical modelization, mathematical analysis of models, and numerical simulation in Science and Technology is nowadays unquestionable. These aspects of Mathematics should be therefore considered as an essential part of education in schools of mathematics and engineering.

The aim of this paper is to provide a didactical proposal to introduce the above mentioned aspects of Applied Mathematics (modelization, mathematical analysis and numerical simulation) to undergraduate engineering students who have received some preliminary courses on linear algebra, calculus, differential equations and numerical analysis.

The paper is organized as follows. Section 2 contains a couple of models which are of particular interest in Engineering and which are matematically formulated as boundary value problems (see [1, 2] for other interesting examples). Although Physics is different in these problems, Mathematics is the same. Section 3 shows that we have to look at these problems with a different eyes rather than the classical ones, that is, there are a number of interesting problems in Engineering which have no *classical* solution. Section 4 is intended to provide the basic mathematical background it is needed to study those models with mathematical rigour. In Section 5 we arrive to the concept of *weak* solution for a boundary value problem and prove the existence, uniqueness and continuous dependence on the initial data for the models considered in Section 2. In Section 6 we pay our attention on numerical analysis and simulation. The aim here is to show the ideas underlying one of the most useful numerical methods in Engineering: the finite element method. In this method we find a wonderful example of a surprising alliance between the new abstract and numerical concepts. Finally, we give a new example of how computers can be integrated in mathematical education. Precisely, we use MATLAB to obtain numerical simulations of the models considered along the paper (see [3] for more information on mathematical education with MATLAB).

2. A Couple of Models Arising in Heat Diffusion and Linear Elasticity

In this section, a couple of simple models which are of particular interest in heat diffusion and linear elasticity are deduced. These models are two of the standard examples to which

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the methods presented in this paper apply. For the sake of clarity and simplicity, only the one-dimensional case is considered although it is necessary to point out that most of the ideas presented in this case follow (along the same lines) in higher dimensions.

Consider a cylindrical rod of length L and assume the length of the rod is much more large than the radius of the cylinder so that we may consider that heat flows only along the $x-$axis. Fourier's law states that the heat flux, say q, is proportional to the gradient of temperature u, that is,

$$q = -\kappa u' \tag{1}$$

where $\kappa = \kappa(x) \geq \kappa_0 > 0$ depends on the physical properties of the material and it is called the *thermal conductivity.* The minus sign in (1) means that heat goes from high to low temperatures. Now consider a small portion $[x_0, x_1]$ of the rod. The heat crossing this portion is given by

$$q(x_1) - q(x_0) = -\kappa(x_1) u'(x_1) + \kappa(x_0) u'(x_0) = \int_{x_0}^{x_1} -(\kappa(x) u'(x))' \, dx. \tag{2}$$

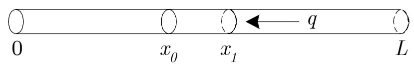


FIGURE 1. Heat diffusion in a rod of length L.

This flux of heat may be produced by an internal source of heat and/or an external one. We denote both contributions of heat by the density function $f = f(x)$, which for simplicity we assume does not depend on time. Hence, along $[x_0, x_1]$ we have

$$\int_{x_0}^{x_1} f(x) \, dx. \tag{3}$$

Conservation of energy leads to

$$\int_{x_0}^{x_1} \left[-(\kappa(x) u'(x))' - f(x) \right] dx = 0$$

and as the above holds for all $0 < x_0 < x < x_1 < L$,

$$-(\kappa(x) u'(x))' = f(x) \quad \text{for all } 0 < x < L.$$

If in addition we assume that the extremes of the rod are insulated, that is, $q(0) = q(L) = 0$, then from (1) it follows that $u'(0) = u'(L) = 0$.

Up to now we have supposed that the rod is insulated along its length. Newton's law of cooling says that heat transfer takes place at a rate proportional to the difference of temperature between the rod and the surroundings (for simplicity we assume that the surroundings hold at zero temperature). From this we obtain the modified stationary heat equation

$$-(\kappa u')' + \lambda u = f \quad \text{in } (0, L)$$

where $\lambda = \lambda(x) \geq \lambda_0 > 0$. To sump up, the mathematical model for the stationary problem of heat diffusion in a rod, with insulated extremes, is given by

$$\text{(HP)} \qquad \begin{cases} -(\kappa u')' + \lambda u = f & \text{in} \quad (0, L) \\ u'(0) = u'(L) = 0 \end{cases}$$

Now consider a perfectly elastic and flexible string stretched along the segment $[0, L]$. Assume that on the string acts a vertical force $f = f(x)$ and that the string is fixed at both endpoints.

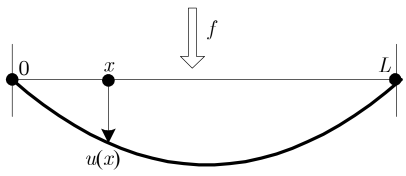


FIGURE 2. String fixed at the endpoints and supporting the force f.

Hooke's law on linear elasticity and the momentum conservation law lead to the equation $-(\kappa u')' = f$ in $(0, L)$, where $\kappa = \kappa(x) \geq \kappa_0 > 0$ depends on the physical properties of the string. If in addition, this experiment occurs in an elastic medium, then it produces a force (which is opposite to f) given by $-\lambda u$, where $\lambda = \lambda(x) \geq \lambda_0 > 0$. Thus, we have

$$-(\kappa u')' + \lambda u = f \quad \text{in } (0, L) \tag{4}$$

and therefore, the mathematical model for this problem is

$$\text{(SP)} \qquad \begin{cases} -(\kappa u')' + \lambda u = f & \text{in} \quad (0, L) \\ u(0) = u(L) = 0 \end{cases}$$

Notice that although the problems of heat diffusion in the rod and the flexion of the string are obviously different, however Mathematics, in both problems, is essentially the same.

Let us go back to the problem of the string. Assume that the external force is located at a point $x = L/2$. It is evident that the position of the string is given as the following figure shows.

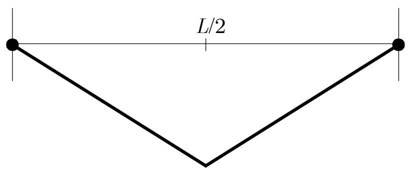


FIGURE 3. String fixed at the endpoints and supporting a charge located at $x = L/2$.

But a function as given in the preceding picture is not differentiable at $x = L/2$. Hence, such as function cannot be a solution of the differential equation $-(\kappa u')' = f$ in $(0, L)$, at least in the classical sense, that is, in the sense of being u twice differentiable at each point of the open interval $(0, L)$ and satisfying the differential equation in that interval. This simple example shows that it is necessary to look for a new way of understanding the concept of a solution of a differential equation.

3. LOOKING FOR A NEW WAY OF UNDERSTANDING THE CONCEPT OF A SOLUTION OF A DIFFERENTIAL EQUATION

Consider again the problem of the string. If the force f produces a virtual displacement $v(x)$ at a point x, then the work produced by $f(x)$ is $f(x)\, v(x)$ so that the work produced by f along the whole string is given by

$$\int_0^L f(x)\, v(x)\ dx.$$

Proceeding in the same way in the left-hand side of (4) and integrating by parts,

$$\int_0^L -\left(\kappa(x)\, u'(x)\right)' v(x)\ dx = \int_0^L \kappa(x)\, u'(x)\, v'(x)\ dx$$

since $v(0) = v(L) = 0$. This process transforms the differential equation $-(ku')' + \lambda u = f$ into the integral equation

$$\int_0^L \kappa(x)\, u'(x)\, v'(x)\ dx + \int_0^L \lambda(x)\, u(x)\, v(x)\ dx = \int_0^L f(x)\, v(x)\ dx. \tag{5}$$

Hence, we may think in a solution of problem (SP) as a function $u : [0, L] \to \mathbb{R}$, with $u(0) = u(L) = 0$, which satisfies (5) for all possible displacements v such that $v(0) = v(L) = 0$. One of the main advantages of this approach is that we have reduced the requirements that the function u ought to satisfy. Nevertheless, there are still two main points which are not clear at all:

(1) u should be at least once differentiable, but this is not the case for a charge located at a point.
(2) if the charge is located at $x = L/2$ (that is, $f(x) = 0$ for all $0 \leq x \leq L$, $x \neq L/2$), then $\int_0^L f(x)\, v(x)\ dx = 0$ so that $u = 0$ satisfies (5), in contradiction with the physical experience (see Figure 3).

The above shows that it is necessary to understand better the way of dealing matematically with the concept of a charge located at a point. As a first approach, let us consider that the charge is distributed in a small portion around $x = L/2$, that is,

$$f_\varepsilon(x) = \begin{cases} 1/(2\varepsilon), & \frac{L}{2} - \varepsilon \leq x \leq \frac{L}{2} + \varepsilon \\ 0, & \text{otherwise} \end{cases}$$

The work produced by this charge with a displacement v is now given by

$$\int_0^L f_\varepsilon(x)\, v(x)\ dx = \int_{\frac{L}{2}-\varepsilon}^{\frac{L}{2}+\varepsilon} \frac{v(x)}{2\varepsilon}\ dx = v(\xi_\varepsilon),$$

where $\frac{L}{2} - \varepsilon \leq \xi_\varepsilon \leq \frac{L}{2} + \varepsilon$, and the equality being a consequence of the mean value theorem for integrals. Now letting $\varepsilon \to 0$ and assuming v is continuous it is concluded that, in this sense, the work produced by a single charge located at $L/2$ and producing a displacement $v = v(x)$ is $v(L/2)$. This reasoning shows that we can deal matematically with a single charge located at a point x_0 as a mapping, say δ_{x_0}, which acts on a certain class of functions and produce numbers by following the rule

$$\delta_{x_0} : v \mapsto < \delta_{x_0}, v > =^{\text{def}} v(x_0).$$

This was the origin of the theory of distributions discovered by the french mathematician L. Schwartz in 1946, and this is basically the mathematical background we need to formulate precisely a boundary value problem.

4. The mathematics we need

In this section it is aimed to show the basic ideas of the mathematics are needed to study a one-dimensional boundary value problem with mathematical rigour.

Given an open interval $I \subseteq \mathbb{R}$, $\mathcal{D}(I)$ stands for the *test functions space* composed of all functions $v : I \to \mathbb{R}$ which are indefinitely differentiable and have compact support[1] in I. Now given a sequence $\{v_n\}_{n=1}^{\infty} \subseteq \mathcal{D}(I)$ it is said that this sequence converges to $v \in \mathcal{D}(I)$ if (i) there exists a compact set $K \subseteq I$ such that supp $v_n \subseteq K$ for all $n \in \mathbb{N}$, and (ii) for each $m \in \mathbb{N}$, $\frac{d^m}{dx^m} v_n$ converges uniformly to $\frac{d^m}{dx^m} v$.

A distribution u is defined as a linear and continuous (with respect to the above notion of convergence) mapping $u : \mathcal{D}(I) \to \mathbb{R}$. Let us now show the two typical examples of distributions.

- If $f : I \to \mathbb{R}$ is locally integrable, then a distribution u_f may be associated with f by means of the mapping
$$u_f : \mathcal{D}(I) \to \mathbb{R}, \quad v \mapsto < u_f, v > =^{\text{def}} \int_I f(x)\, v(x)\ dx.$$
It is very common to denote by f the distribution u_f. In what follows we use this notation.
- Given $x_0 \in I$, it is not hard to show that the mapping
$$\delta_{x_0} : \mathcal{D}(I) \to \mathbb{R}, \quad v \mapsto < \delta_{x_0}, v > =^{\text{def}} v(x_0)$$
is a distribution. This distribution is called the Dirac delta.

Next, we wish to do calculus with distributions. In particular, we wonder if it is possible to define the derivative of a distribution. Assume first that $f : I \to \mathbb{R}$ is a differentiable function and take $v \in \mathcal{D}(I)$. From the distributions point of view, the derivative of f is given by $\int f'v$, but integrating by parts and taking into account that v vanishes at the extremes of I it is concluded that $\int f'v = -\int fv'$, that is, in the language of distributions

$$< f', v > = - < f, v' > .$$

In general, given a distribution u, its distributional derivative is defined as the distribution u' given by

$$< u', v > = - < u, v' > \quad \text{for all } v \in \mathcal{D}(I). \tag{6}$$

Notice that, contrary to what happens with functions, a distribution may be derived infinitely times. Let us show a concrete example.

Example 1. *Consider the function*

$$u(x) = \begin{cases} -\frac{x}{2}, & 0 \le x \le 1/2 \\ \frac{x}{2} - \frac{1}{2}, & 1/2 \le x \le 1 \end{cases}$$

Since u is locally integrable, it may be considered as a distribution. From (6) and integrating by parts it is not hard to show that u' is the distribution associated with the function

$$u'(x) = \begin{cases} -1/2, & 0 \le x < 1/2 \\ 1/2, & 1/2 < x \le 1 \end{cases}$$

and derivating again it is concluded that $u'' = \delta_{1/2}$, in the sense of distributions.

[1] the support of a continuous function v is defined as supp $v = \overline{\{x \in I : v(x) \neq 0\}}$.

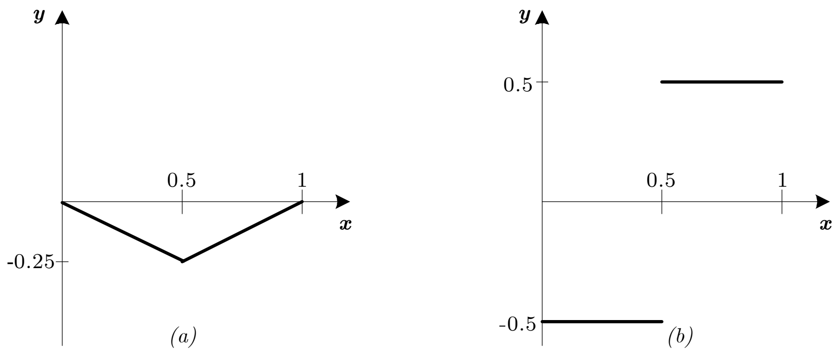


FIGURE 4. In (a) it is shown the function u, and in (b) its distributional derivative.

5. Mathematical Analysis of Models: the Variational Method

Once we have at one's disposal distributions, let us go back to (SP) or in particular to the integral equation (5). Let $L^2(0,L)$ denote the Hilbert space of functions $f:(0,L)\to\mathbb{R}$ of square integrable endowed with the norm $\|f\|_2=\left(\int_0^L f^2(x)\,dx\right)^{1/2}$. In order to the right-hand side of (5) to make sense, by the Cauchy-Schwarz inequality, all we need is to have $f,v\in L^2$. As for the left-hand side of (5), if we assume κ and λ to be bounded, then we just need $u,v,u',v'\in L^2$, that is, that u,v and its derivatives (in the sense of distributions) to be in L^2. For instance, the function u and its derivative u' as given in Example 1 are in L^2. As usual, we denote by

$$H_0^1(0,L)=\left\{u\in L^2(0,L):u'\in L^2(0,L),\ u(0)=u(L)=0\right\},$$

which endowed with the norm $\|u\|_{H_0^1}=\left(\|u\|_2^2+\|u'\|_2^2\right)^{1/2}$ is a Hilbert space. Of course, the derivatives in this space are understood in the sense of distributions. It can be proved that the test functions space $\mathcal{D}(0,L)$ is $\|\cdot\|_{H_0^1}-$dense in $H_0^1(0,L)$. From this it follows that the Dirac delta can be extended to a linear and continuous form $\delta_{x_0}:H_0^1(0,L)\to\mathbb{R}$, acting as $<\delta_{x_0},u>=u(x_0)$, with $u\in H_0^1$. Functions f of L^2 may be also considered as linear and continuous forms on H_0^1 just by defining it as

$$f:H_0^1\to\mathbb{R},\quad v\mapsto <f,v>=^{\text{def}}\int fv.$$

These new ideas lead to a new formulation of (SP). Precisely, given a linear and continuous form $f:H_0^1\to\mathbb{R}$ and the bilinear form

$$a:H_0^1\times H_0^1\to\mathbb{R},\quad (u,v)\mapsto a(u,v)=\int_0^L\kappa(x)\,u'(x)\,v'(x)\ dx+\int_0^L\lambda(x)\,u(x)\,v(x)\ dx$$

a function $u\in H_0^1$ is said to be a *weak solution* of (SP) if the identity

$$a(u,v)=<f,v>$$

holds for all $v\in H_0^1$.

The above may be put in a more general setting (which is very useful in practice as we shall see later on) as follows:

Definition 1 (Variational Problem)**.** *Given a Hilbert space* $(H, \|\cdot\|)$, *a linear and continuous form* $f : H \to \mathbb{R}$, *and a bilinear form* $a : H \times H \to \mathbb{R}$, *by variational problem we mean the problem of finding* $u \in H$ *such that*

$$\text{(VP)} \qquad a(u,v) =< f, v > \quad \textit{for all } v \in H.$$

Such a function $u \in H$ *is called a weak solution of (VP).*

Existence, uniqueness and continuous dependence on the initial data of weak solutions for (VP) is obtained through one of the most beautiful and useful theorems in Applied Mathematics: the Lax-Milgram Theorem. For the proof we refer to [4, p. 297].

Theorem 1 (Lax-Milgram)**.** *If the bilinear form* $a(\cdot,\cdot)$ *is continuous (that is, there exists* $M > 0$ *such that* $|a(u,v)| \leq M \|u\| \|v\|$ *for all* $u, v \in H$*) and coercitive (this means that there exists* $m > 0$ *such that* $a(u,u) \geq m \|u\|^2$ *for all* $u \in H$*), then the variational problem (VP) has a unique weak solution. Moreover,*

$$\|u\| \leq \frac{1}{m} |||f||| ,$$

where $|||f||| =^{def} \sup \{|< f, v >| , \ v \in H, \ \|v\| \leq 1\}$.

As we mentioned before, this abstract version of a boundary value problem is very useful in practice. For instance, for (SP) me must take $H = H_0^1$. Proceeding in the same way with the heat diffusion problem (HP), that is, multiplying the differential equation by a function v, integrating by parts, and taking into account the boundary conditions $u'(0) = u'(L) = 0$, then we easily find that the space where we ought to look for a solution is

$$H^1(0,L) = \left\{ u \in L^2 : u' \in L^2 \right\},$$

which endowed with the same norm as H_0^1 is a Hilbert space. Hence, the variational formulation of (HP) consists of looking for a function $u \in H^1$ such that

$$a(u,v) =^{\text{def}} \int_0^L \kappa(x) u'(x) v'(x) \ dx + \int_0^L \lambda(x) u(x) v(x) \ dx =< f, v > \quad \text{for all } v \in H^1.$$

As for the hypothesis of the Lax-Milgram theorem, the continuity of $a(\cdot,\cdot)$ is a consequence of the Cauchy-Schwartz inequality, and coercivity follows from the estimate

$$a(u,u) = \int_0^L \kappa(x) (u')^2(x) \ dx + \int_0^L \lambda(x) u^2(x) \ dx \geq \min\{\kappa_0, \lambda_0\} \|u\|_{H_0^1}^2$$

Nevertheless, the most difficult hypothesis of the Lax-Milgram theorem to check in practice is coercitivity. For instance, for the (SP) problem with $\lambda = 0$, coercitivity follows from the Poincaré inequality (see [4, Th. 3, p. 265]).

6. Numerical Simulation of Weak Solutions: the Finite Element Method

In the preceding section we have developed the basic ideas to prove the existence and uniqueness of weak solutions for a boundary value problem. However, this is not enough in Engineering. We must find the solution of our problem, or at least, a numerical approximation of the solution. This section is intended to show the ideas underlying one of the most useful numerical methods in Engineering: the finite element method (FEM).

We already know that our solution lives in a Hilbert space H such as H^1 or H_0^1. The main difficulty is that these spaces are too big. Precisely, they are infinite-dimensional. The basic idea of the FEM consists of approximating the big space H by some appropriate finite-dimensional spaces H_h, where h is a positive parameter, satisfying the following conditions:

(a) $H_h \subseteq H$,
(b) in H_h we can easily solve the variational problem and hence obtain a solution u_h, and
(c) when $h \searrow 0$, $H_h \nearrow H$, or in other words, $\lim_{h\to 0} \|u - u_h\| = 0$.

This procedure leads to a numerical approximation u_h of the weak solution u of our original problem. Let us show how this method works for the case of the (SP) problem.

Construction of H_h

Let $n \in \mathbb{N}$ and $h = 1/(n+1)$. The interval $[0, L]$ can be decomposed as

$$[0, L] = \bigcup_{i=0}^{n} [c_i, c_{i+1}], \quad c_i = ih, \ 0 \leq i \leq n.$$

Now set

$$H_h = \left\{ v : [0, L] \to \mathbb{R} \text{ continuous, } v(0) = v(L) = 0 \text{ and } v|_{[c_i, c_{i+1}]} \in \mathcal{P}_1 \right\}$$

where $\mathcal{P}_1$ stands for the space of polynomials of degree less than or equal to 1. It is not hard to show that $H_h \subseteq H_0^1$. As for the dimension of H_h, the family of functions

$$\phi_i(x) = \begin{cases} 1 - \frac{|x - c_i|}{h}, & c_{i-1} \leq x \leq c_{i+1} \\ 0, & \text{otherwise} \end{cases}$$

for $1 \leq i \leq n$, is a basis of H_h. Therefore, $dim(H_h) = n$.

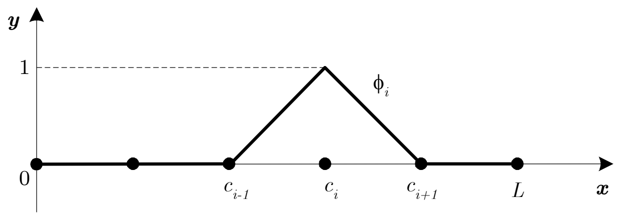


FIGURE 5. A function ϕ_i of the basis of H_h.

The construction of the space H_h is not unique. Other options are possible as well. Anyway, we are considering here the simplest case.

The variational problem in H_h

Since $H_h \subseteq H_0^1$ is finite-dimensional, $\left(H_h, \|\cdot\|_{H_0^1}\right)$ is a Hilbert space. Thus, the variational problem (SP) in H_h is formulated as follows: find $u_h = \sum_{i=1}^{n} u_h^i \phi_i \in H_h$ such that the identity

$$a(u_h, v_h) =^{\text{def}} \int_0^L \kappa u_h' v_h' + \int_0^L \lambda u_h v_h = < f, v_h > \tag{7}$$

holds for all $v_h \in H_h$. Remember that if $f \in L^2$, then $< f, v_h >= \int_0^L f v_h$; and if f is a Dirac delta at x_0, then $< f, v_h >= v_h(x_0)$.

It is evident that if (7) holds for all $v_h \in H_h$, then it is held for all ϕ_i, $1 \leq i \leq n$; and conversely, since H_h is a vector space, if (7) holds for all ϕ_i, $1 \leq i \leq n$, then it is held for all $v_h \in H_h$. Hence, the integral equation (7) transforms into the linear system

$$\sum_{i=1}^{n} u_h^i a\left(\phi_i, \phi_j\right) =< f, \phi_j >, \quad 1 \leq j \leq n$$

and taking into account the properties of the functions ϕ_i, this system is written as

$$\begin{cases} a\left(\phi_1, \phi_1\right) u_h^1 + a\left(\phi_2, \phi_1\right) u_h^2 + 0 & = \quad < f, \phi_1 > \\ \dots\dots\dots\dots\dots & \dots \quad \dots \\ 0 + a\left(\phi_{i-1}, \phi_i\right) u_h^{i-1} + a\left(\phi_i, \phi_i\right) u_h^i + a\left(\phi_{i+1}, \phi_i\right) u_h^{i+1} + 0 & = \quad < f, \phi_i > \\ \dots\dots\dots\dots\dots & \dots \quad \dots \\ 0 + a\left(\phi_{n-1}, \phi_n\right) u_h^{n-1} + a\left(\phi_n, \phi_n\right) u_h^n & = \quad < f, \phi_n > \end{cases}$$

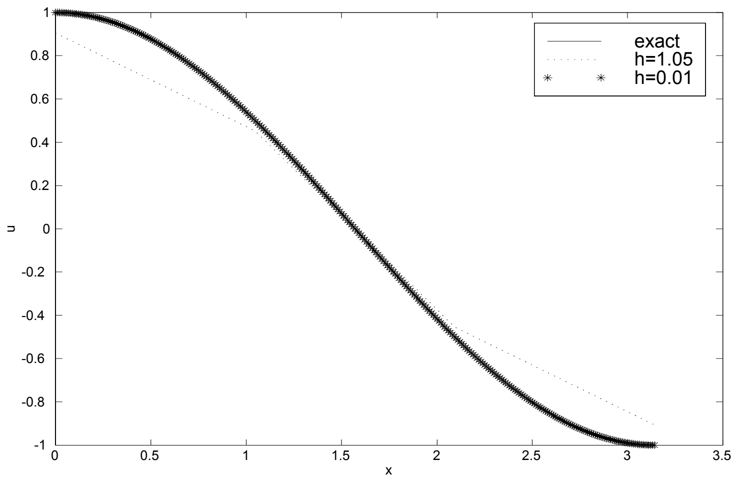
Note that since the matrix of this system is three-diagonal, a numerical method for linear systems such as the Cholesky method is suitable to solve it. As for the computation of the integrals in $a\left(\phi_i, \phi_j\right)$ and in $< f, \phi_i >$, this may be done by the mid-point rule.

Numerical experiments

Next we show how to use MATLAB to obtain a numerical approximation of the weak solutions of the heat diffusion problem (HP) and the string problem (SP). We do not aim to do a complete analysis of the possibilities of MATLAB in boundary value problems. This would be a topic for an specific paper. We just present a couple of numerical experiments.

A code based on the FEM is developed in MATLAB for solving boundary value problems in two dimensions. For the one-dimensional case, a number of textbooks provide a floppy disk where this code is developed as well. This is the case of [5, pp. 268-269] where a code of finite elements for the one-dimensional case (which follows the ideas developed in the preceding section) is presented in the `elfin.m` file. We refer to that reference to the interested reader.

Consider the heat problem (HP) with $L = \pi$, $\kappa = \lambda = 1$ and $f(x) = 2\cos x$. This problem has a exact solution given by $u(x) = \cos x$. Using the `elfin.m` file we obtain the results as given in the next figure.



This picture shows the weak solution $u(x) = \cos x$ and two numerical approximations. The first one corresponds to take $h = 1.05$, and the second one to $h = 0.01$. We are not able to distinguish between the exact solution and the one corresponding to $h = 0.01$. This is due to the fact that both solutions are very close. To be precise, we may compute de error between both solutions at the mesh points c_i by using the function `norm` of MATLAB, which gives us the sup norm. We obtain that this error is equal to $8.3418e - 006$, which is a very good approximation.

Finally, consider the string problem (SP) with $L = 1$, $\kappa = 1$, $\lambda = 0$ and $f = -\delta_{1/2}$. A slight modification of the `elfin.m` file is needed to introduce the elements $< -\delta_{1/2}, \phi_i >= -\phi_i\,(0.5)$. The results are presented in the next figure.

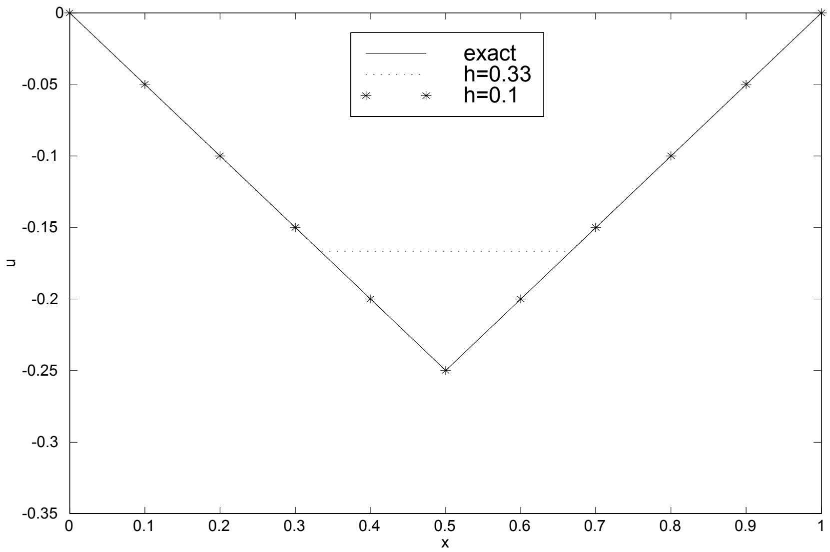


FIGURE 6. Numerical aproximations of the weak solution of (SP).

This is the end of our journey. For the reader interested in the finite element method we refer, for instance, to [6].

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