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Terceras Jornadas sobre Ecuaciones Diferenciales, Optimización y Análisis Numérico

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TERCERAS JORNADAS SOBRE ECUACIONES DIFERENCIALES, OPTIMIZACIÓN Y ANÁLISIS NUMÉRICO

Maria Cristina Maciel - Domingo Alberto Tarzia (Eds.)

INDICE

Rosario, Marzo 2007

Las Terceras Jornadas sobre Ecuaciones Diferenciales, Optimización y Análisis Numérico tuvieron lugar en el Departamento de Matemática de la Universidad Nacional del Sur, en la ciudad de Bahía Blanca, del 9 al 10 de Marzo de 2006. Fue realizado con el apoyo del Proyecto de Investigación Plurianual "Partial Differential Equations and Numerical Optimization with Applications" subsidiado por la Fundación Antorchas e integrado por los siguientes subproyectos:

- "Free Boundary Problems for the Heat-Diffusion Equation" (UA-UNR-UNRC-UNSa);
- "Inverse and Control Problems in the Mathematical Modeling of Phase Transitions in Shape Memory Alloys" (UNL);
- "Geophysical Scale Stratified Flows and Hydraulic Jumps" (UNC-UBA-UNLPa);
- "Optimization Applied to Mechanical Engineering Problems" (UNS-UNC-UNCo).

El Comité Organizador estuvo compuesto por: M.C. Maciel (Bahía Blanca, Coordinadora), R.D. Spies (Santa Fe), D. A. Tarzia, (Rosario); C.V. Turner (Córdoba). La Secretaría Local estuvo compuesta por: Gabriela Eberle, Tatiana Gibelli y Adriana Verdiell (Coordinadora).

Las Jornadas estuvieron dirigidas a graduados, profesionales y estudiantes de Matemática, Física, Química, Ingeniería y ramas afines, con conocimientos básicos sobre ecuaciones diferenciales, análisis numérico y optimización.

En MAT – Serie A, # 14 (2007) se publican cinco de las conferencias y comunicaciones presentadas. Los manuscritos fueron recibidos y aceptados en marzo de 2007.

CONFERENCIAS Y COMUNICACIONES DE LAS TERCERAS JORNADAS SOBRE ECUACIONES DIFERENCIALES, OPTIMIZACIÓN Y ANÁLISIS NUMÉRICO

Jueves 9 de marzo de 2006

- Gabriela Eberle (Bahía Blanca), "Método de Newton en espacios matriciales".
- Adriana Verdiell (Bahía Blanca), "Manejo de áreas naturales: alcances y limitaciones de un modelo matemático".
- María Cristina Maciel (Bahía Blanca), "Aplicación de la condición PLD al problema de optimización multiobjetivo".
- Olga Emilia Mandrini (Neuquén), "Sobre la resolución numérica de un problema de optimización de formas".
- Tatiana Gibelli (Bahía Blanca), "Un algoritmo para minimización de función lineal con restricciones cuadráticas convexas".
- María Cristina Sanziel (Rosario), "Optimización del flujo total de calor en un problema con restricciones de temperatura, a través de un problema de Cauchy para la ecuación de Laplace".
- Mariela C. Olguin (Rosario), "Comportamiento monótono de la temperatura y la frontera libre de una sustancia, respecto de la variación de sus coeficientes térmicos".
- Domingo A. Tarzia (Rosario), "La ecuación del calor no-clásica. Solución explícita para un problema de Stefan con dato de temperatura en el borde fijo".
- Eduardo A. Santillan Marcus (Rosario), "Un problema de desublimación en un medio poroso húmedo".

Viernes 10 de marzo de 2006:

- Rubén Spies (Santa Fe), "Sobre un modelo termoelástico para los movimientos de las antenas del Telescopio espacial James Webb".
- Karina Temperini (Santa Fe), "Divergencia con velocidad arbitraria del método de mínimos cuadrados en problemas inversos mal condicionados".
- Jorge L. Blengino (Río Cuarto), "Toma de agua por raíces de cultivos. Algunos resultados numéricos".
- Juan C. Reginato (Río Cuarto), "Interaccciones en la toma de nutrientes. Uso de cinéticas competitivas en un modelo de frontera móvil".
- Marcos Gaudiano (Córdoba), "Condición convectiva en la difusión de un solvente en un polímero vidrioso".

LARGE-SCALE ALGORITHMS FOR MINIMIZING A LINEAR FUNCTION WITH A STRICTLY CONVEX QUADRATIC CONSTRAINT[1]

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Abstract

The problem of minimizing a linear function subject to convex quadratic constraints appears in many topological optimization problems such as truss and free material optimization. Usually this kind of problems is solved using interior point methods. In this work, the problem with only one constraint is considered. The solution of the problem is analyzed when the constraint matrix is symmetric and positive definite. A simple iterative algorithm is proposed. It is essentially based on the steepest descent direction and the geometric properties of the problem. In this method an iteration goes to the boundary in the negative gradient direction and then it finds the center of the region determined by the intersection of the level hyperplane and the feasible set. The convergence of this algorithm is analyzed. Also, an improved version of the algorithm is established. It comes from the observation that centers are in the same line, so only one center-finding operation is needed. Because of its simplicity, these algorithms are appropriate for very large scale problems. Numerical results are presented.

Key words: Quadratic Constraints, Topological Optimization.
AMS Subject Classification: 49M40, 49N10, 90C25, 90C30.

1 Introduction

Some topologic optimization problems, like truss and free material optimization, can be established as a constrained optimization problem as follows

$$\begin{array}{ll} \min\limits_{s.t.} & c^T x \\ & \frac{1}{2} x^T A_i x \leq b_i, \quad i = 1, ..., m, \end{array} \tag{1}$$

where $c \in \mathbb{R}^n$, $A_i \in \mathbb{R}^{n \times n}$ are symmetric positive semidefinite matrices, and $b_i \in \mathbb{R}$ for all $i = 1, ..., m$ [3].

This kind of problems belongs to the more general class of convex optimization problems:

$$\begin{array}{ll} \min\limits_{s.t.} & f(x) \\ & g_i(x) \leq 0, \quad i = 1, ..., m, \end{array} \tag{2}$$

where $f, g_i : \mathbb{R}^n \to \mathbb{R}$ are twice continuously differentiable convex functions, the set of optimal solutions is a nonempty and compact set and there exists a point $\widehat{x}$ such as $g_i(\widehat{x}) < 0$ for all $i = 1, ..., m$.

Many numerical methods solve the problem under some additional assumptions. The interior point methods are perhaps the most popular [1, 4, 6, 10]. They are used to transform a

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constrained problem to a sequence of unconstrained problems, which are solved via well known algorithms, for instance the Newton method. Ben-Tal and Zibulesvsky [2] have developed an efficient method for large scale convex problems which are very common in topological design. The algorithm combines ideas of penalty and barrier methods with the Augmented Lagrangian method.

In this work, the problem (1) is analyzed with only one quadratic constraint, and the matrix is symmetric and positive definite. First, the existence of solution and its exact expression is studied. Then, according to the geometric characteristics of the problem an iterative algorithm is proposed to find the solution. The convergence of this algorithm is analyzed. Finally, an improved version of the algorithm is presented and some numerical results are shown to illustrate the behavior of the algorithms.

2 The problem

We consider the optimization problem

$$\begin{array}{ll} \min\limits_{s.t.} & f(x) = c^T x \\ & \dfrac{1}{2} x^T A x - d^T x \leq b, \end{array} \tag{3}$$

where $c \in \mathbb{R}^n$, $c \neq 0$, $d \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$ is a symmetric positive definite matrix and $b \in \mathbb{R}$, $b > 0$.

The problem (3) can be transformed into the following one

$$\begin{array}{ll} \min\limits_{s.t.} & c^T x \\ & \dfrac{1}{2} x^T A x \leq b, \end{array} \tag{4}$$

via a simple substitution. Such a substitution consists of translating the center of the quadratic $\frac{1}{2} x^T A x - d^T x = b$ to the origin.

The proposed algorithm is based on the geometric properties of the last problem. We state some of them.

Lemma 2.1 *The problem (4) has a unique solution x^* and it satisfies that Ax^* and c are parallel directions.*

Proof: It is straightforward. □

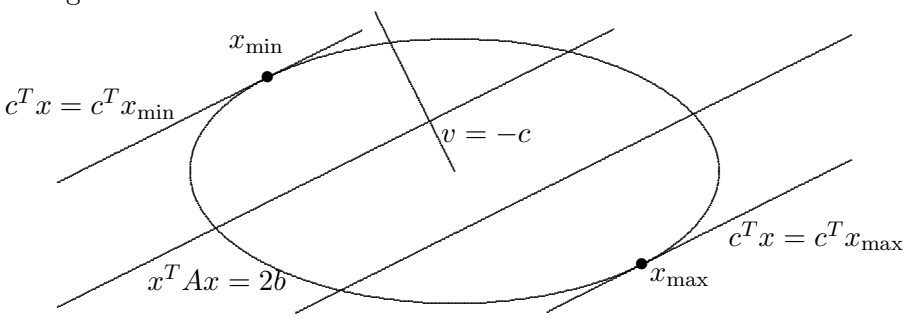

Figure 1: The geometric properties of the problem

Lemma 2.2 *The problem (4), where $c \in \mathbb{R}^n$, $c \neq 0$, $A = I_n$, and b is a positive real number, has a unique solution $x^* = -\sqrt{\dfrac{2b}{c^T c}}\, c$.*

Proof: It is straightforward. □

Theorem 2.1 *The problem (4) has a unique solution,* $x^* = -\sqrt{\dfrac{2b}{c^T A^{-1} c}}\, A^{-1} c$.

Proof: It follows from Lemma 2.1. □

3 The algorithm

The exact solution of problem (4) requires the computation of the inverse matrix of A. It is well known that this computation is not convenient because of the numerical errors and the arithmetic cost. Then, we propose an iterative method which does not require the inverse matrix of A and takes into account the geometric properties of the problem described above.

The main idea is to find alternatively an interior point and a border point following the steepest descent direction of the objective function until the minimizer is reached. The algorithm starts with an interior point. Without of generality, let us take $y_1 = 0$.

Figure 2 shows the sequence of interior and border points generated by this algorithm.

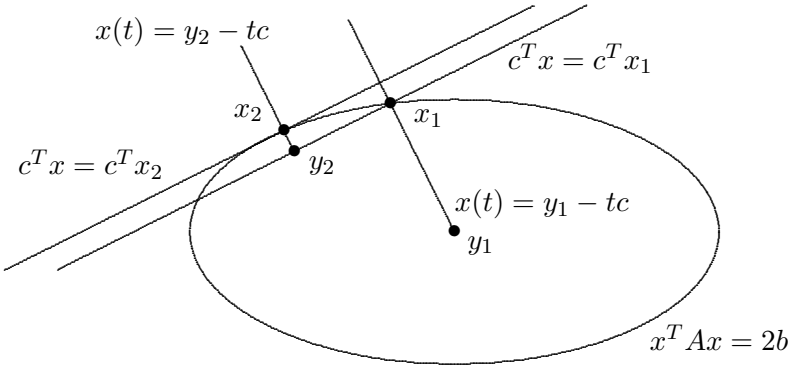

Figure 2: The behavior of the iterative method

Algorithm 1:
Given: $c \in \mathbb{R}^n,\ c \neq 0,\ A \in \mathbb{R}^{n\times n}$ symmetric and positive definite matrix and $b \in \mathbb{R},\ b > 0$.
For $k = 1, 2, \ldots$. "until convergence" repeat

Step 1:

- If $k = 1$, $y_1 = 0$.
- If $k > 1$, find an interior point y_k as the center of the resulting intersection between the level hyperplane $c^T x = c^T x_{k-1}$ and the constraint.

Step 2: Find a border point x_k as the intersection between the halfline passing through y_k in the direction $v = -c$ and the constraint.

Now let us describe in details Step 1 and 2.

- **Step 1:** $(k > 1)$ Since $c \neq 0$, there exists at least an index i such that $c_i \neq 0$. If $f_{k-1} = c^T x_{k-1}$, then from the hyperplane $c^T x = f_{k-1}$ it is possible to obtain the component

$$x_i = \frac{1}{c_i}\left(f_{k-1} - \sum_{j\neq i,\ j=1}^{n} c_j\, x_j\right).$$

Then,

$$\begin{pmatrix} x_1 \\ \vdots \\ x_{i-1} \\ x_i \\ x_{i+1} \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} 1 & 0 & \dots & \dots & 0 & 0 \\ 0 & 1 & \dots & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\frac{c_1}{c_i} & \dots & -\frac{c_{i-1}}{c_i} & -\frac{c_{i+1}}{c_i} & \dots & -\frac{c_n}{c_i} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \dots & 1 & 0 \\ 0 & 0 & \dots & \dots & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_{i-1} \\ x_{i+1} \\ \vdots \\ x_n \end{pmatrix} + \frac{f_{k-1}}{c_i} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Let

- $P \in \mathbb{R}^{n\times(n-1)}$ be the matrix obtained from the identity $I_{n-1} \in \mathbb{R}^{(n-1)\times(n-1)}$ adding the zero vector as the i-th row . Clearly $PP^T = I_n$ and $P^TP = I_{n-1}$.
- $e = \dfrac{e_i}{c_i}$, where $e_i^T = (0, 0, ..., \underset{\text{place } i}{1}, ..., 0, 0) \in \mathbb{R}^n$.

So $x = B\widehat{x} + f_{k-1}e$ where $B = (I_n - ec^T)P \in \mathbb{R}^{n\times(n-1)}$ and $\widehat{x} = P^Tx \in \mathbb{R}^{n-1}$. The intersection between the hyperplane $x = B\widehat{x} + f_{k-1}e$ with the constraint $\frac{1}{2}x^TAx = b$ is

$$\frac{1}{2}(B\widehat{x} + f_{k-1}e)^TA(B\widehat{x} + f_{k-1}e) = b$$

$$\frac{1}{2}\widehat{x}^TB^TAB\widehat{x} + f_{k-1}e^TAB\widehat{x} + \frac{1}{2}f_{k-1}^2e^TAe = b$$

$$\frac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d}_k^{\,T}\widehat{x} = \widehat{b}_k,$$

where $\widehat{A} = B^TAB$, $\widehat{d_k} = -f_{k-1}B^TAe$ y $\widehat{b}_k = b - \frac{1}{2}f_{k-1}^2e^TAe$.

The center $\widehat{y}_k$ of $\frac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d}_k^{\,T}\widehat{x} = \widehat{b}_k$ can be obtained by solving the linear system $\widehat{A}x = \widehat{d_k}$ or equivalently by obtaining the minimizer of the quadratic function $\frac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d}_k^{\,T}\widehat{x}$. Clearly, that point can be obtained via any minimization algorithm.

Finally, $y_k = B\widehat{y}_k + f_{k-1}e$.

- **Step 2:** The point x_k is obtained as the intersection between the halfline $x(t) = y_k - tc$, $t > 0$, and the quadratic constraint $x^TAx = 2b$. Then,

$$(y_k - tc)^TA(y_k - tc) = 2b$$

$$y_k^TAy_k - 2tc^TAy_k + t^2c^TAc = 2b$$

$$(c^TAc)t^2 + 2(-c^TAy_k)t + (y_k^TAy_k - 2b) = 0$$

$$t_k = \frac{c^TAy_k + \sqrt{(c^TAy_k)^2 - (c^TAc)(y_k^TAy_k - 2b)}}{c^TAc}$$

$$x_k = y_k - t_kc.$$

- **Stopping criterion:** the termination rules to stop the algorithm are the following:
  - if the closeness between interior and border points is less or equal to a given tolerance $\dfrac{\|y_k - x_k\|}{\|x_k\|} \leq$ tolerance, or

– if the closeness between iterates, $\dfrac{\|x_{k-1} - x_k\|}{\|x_k\|} \leq$ tolerance.

After these considerations, **Algorithm 1** can be written as

Algorithm 1:

Given: $c \neq 0 \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$ symmetric and positive definite and $b \in \mathbb{R}$, $b > 0$.

Compute: B, e, $\widehat{A} = B^T AB$ and $v = B^T Ae$.

For $k = 1, 2, ...$ "until convergence" repeat

Step 1:

- If $k = 1$, $y_1 = 0$.
- If $k > 1$,
  - compute: $f_{k-1} = c^T x_{k-1}$ and $\widehat{d_k} = -f_{k-1}v$.
  - $\widehat{y}_k = argmin\ \dfrac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d_k}^T\widehat{x}$.
  - $y_k = B\widehat{y}_k + f_{k-1}e$.

Step 2:

- $t_k = \dfrac{c^T Ay_k + \sqrt{(c^T Ay_k)^2 - (c^T Ac)(y_k^T Ay_k - 2b)}}{c^T Ac}$.
- $x_k = y_k - t_k c$.

4 Convergence of the algorithm

In this section the behavior of the sequences of interior and border points, $\{y_k\}$ and $\{x_k\}$, generated by the algorithm is analyzed. It will be show that both sequences converge to the solution of the problem (4).

Lemma 4.1 *Let $\{f_k\}$, with $f_k = c^T x_k$ and $\{y_k\}$, the sequences generated by Algorithm 1, and $x^* = -\sqrt{\dfrac{2b}{c^T A^{-1}c}}A^{-1}c$ the solution of problem (4), then*

i) $\{f_k\}$ is a negative decreasing sequence.

$$0 > f_1 > f_2 > ... > f_{k-1} > f_k > f_{k+1} > ...$$

ii) Each term y_k belongs to the halfline $x(t) = t(I_n - B\widehat{A}^{-1}B^T A)e, \quad t < 0$.

iii) $x^{*T}Ax^* = 2b$.

iv) x^* is located to the line $x(t) = t(I_n - B\widehat{A}^{-1}B^T A)e, \quad t < 0$.

Proof:

i) Since $x_1 = -\sqrt{\dfrac{2b}{c^T Ac}}\, c$. Then,

$$f_1 = c^T x_1 = -\sqrt{\frac{2b}{c^T Ac}}\, c^T c < 0.$$

On the other hand, for all k, y_k belongs to the hyperplane $c^T x = c^T x_{k-1}$. Then $c^T y_k = c^T x_{k-1}$. Since $x_k = y_k - t_k c$ with $t_k > 0$ we obtain,

$$f_k = c^T x_k = c^T y_k - t_k c^T c < c^T y_k = c^T x_{k-1} = f_{k-1}.$$

ii) For any iteration k, $\widehat{y}_k = argmin \;\; \frac{1}{2}\widehat{x}^T \widehat{A}\widehat{x} - \widehat{d_k}^T \widehat{x}$, where $\widehat{d_k} = -f_{k-1} B^T Ae$. Therefore, $\widehat{y}_k = \widehat{A}^{-1}\widehat{d_k} = -f_{k-1}\widehat{A}^{-1} B^T Ae$. Since $y_k = B\widehat{y}_k + f_{k-1}e$, it can be written

$$y_k = -f_{k-1} B\widehat{A}^{-1} B^T Ae + f_{k-1}e = f_{k-1}(I_n - B\widehat{A}^{-1} B^T A)e.$$

Therefore for all k, y_k lies on the halfline $x(t) = t(I_n - B\widehat{A}^{-1} B^T A)e$ with $t = f_{k-1} < 0$.

iii) It is straightforward, because

$$x^{*T} Ax^* = (-\sqrt{\frac{2b}{c^T A^{-1} c}} A^{-1} c)^T A(-\sqrt{\frac{2b}{c^T A^{-1} c}} A^{-1} c) = \frac{2b}{c^T A^{-1} c} c^T A^{-1} c = 2b.$$

iv) Let us consider the halfline $x(t) = t(I_n - B\widehat{A}^{-1} B^T A)e$ with $t < 0$ and $t^* = c^T x^*$. Then,

- $t^* < 0$, because

$$t^* = c^T x^* = c^T(-\sqrt{\frac{2b}{c^T A^{-1} c}} A^{-1} c) = -\sqrt{\frac{2b}{c^T A^{-1} c}} c^T A^{-1} c = -\sqrt{2b\, c^T A^{-1} c} < 0.$$

- $x^* = t^*(I_n - B\widehat{A}^{-1} B^T A)e$, because the facts $B = (I_n - ec^T)P$ and $e^T c = 1$ imply that $B^T Ax^* = 0$:

$$\begin{aligned} B^T Ax^* &= -\sqrt{\frac{2b}{c^T A^{-1} c}} B^T c = -\sqrt{\frac{2b}{c^T A^{-1} c}} P^T (I_n - ce^T)c \\ &= -\sqrt{\frac{2b}{c^T A^{-1} c}} P^T (c - c\, e^T c) = -\sqrt{\frac{2b}{c^T A^{-1} c}} P^T (c - c) \\ &= 0. \end{aligned}$$

Then $\widehat{A} P^T x^* = -B^T Aec^T x^*$, because

$$\begin{aligned} \widehat{A} P^T x^* &= B^T ABP^T x^* = B^T A(I_n - ec^T)PP^T x^* \\ &= B^T Ax^* - B^T Aec^T x^* \\ &= -B^T Aec^T x^*. \end{aligned}$$

Therefore, $\widehat{A}^{-1} B^T Aec^T x^* = -P^T x^*$, and

$$\begin{aligned} t^*(I_n - B\widehat{A}^{-1} B^T A)e &= (I_n - B\widehat{A}^{-1} B^T A)ec^T x^* = ec^T x^* - B(\widehat{A}^{-1} B^T Aec^T x^*) \\ &= ec^T x^* + (I_n - ec^T)PP^T x^* = ec^T x^* + x^* - ec^T x^* \\ &= x^*. \end{aligned}$$

□

We establish the convergence result.

Theorem 4.1 *The sequences $\{y_k\}$ and $\{x_k\}$ generated by Algorithm 1 converge to x^*.*

Proof: Since A is symmetric and positive definite, it is possible to consider the elliptic norm $\|z\|_A = \sqrt{z^T A z}$. In first place we show that the sequence $\{\|y_k\|_A\}$ is increasing and upper bounded.

- Since for all k, y_k is an interior point of the feasible region, $\|y_k\|_A^2 = y_k^T A y_k < 2b$. Therefore, the sequence $\{\|y_k\|_A\}$ is upper bounded by $\sqrt{2b}$.
- According to the second part of the Lemma 4.1, $\|y_k\|_A = |f_{k-1}|\|(I_n - B\widehat{A}^{-1}B^T A)e\|_A$ and from the part i) of Lemma 4.1, the sequence $\{|f_k|\}$ is monotone increasing, then the sequence $\{\|y_k\|_A\}$ also results to be monotone increasing.

Therefore, the sequence $\{\|y_k\|_A\}$ is convergent and from the fact that $\{y_k\}$ is contained in a halfline, the sequence $\{y_k\}$ is also convergent. For each k, let us consider the triangle determined by y_k, y_{k+1} and x_k, which is rectangle at x_k. Then

$$\|x_k - y_k\|_2 < \|y_{k+1} - y_k\|_2.$$

The convergence of the sequence $\{y_k\}$ implies

$$\lim_{k\to\infty} x_k = \lim_{k\to\infty} y_k.$$

Moreover, from $\|x_k\|_A = \sqrt{2b}$ for all k, then

$$\lim_{k\to\infty} \|y_k\|_A = \lim_{k\to\infty} \|x_k\|_A = \sqrt{2b}.$$

According to Lemma 4.1 ii), iii) and iv), both x^* and the sequence $\{y_k\}$ are on the halfline passing through the origin and verify $\|y_k\|_A < \sqrt{2b} = \|x^*\|_A$. Thus,

$$\lim_{k\to\infty} \|y_k - x^*\|_A \leq \lim_{k\to\infty} (\|x^*\|_A - \|y_k\|_A) = \sqrt{2b} - \lim_{k\to\infty} \|y_k\|_A = 0.$$

Therefore $\{y_k\}$ converges to x^*, and

$$\lim_{k\to\infty} x_k = \lim_{k\to\infty} y_k = x^*.$$

□

5 Improved version of the algorithm

The Lemma 4.1 suggests a way to simplify the algorithm. Since the interior points generated by the algorithm lie on a line, it is possible to find such a line using two of them. The solution of problem (4) can be found as the intersection of the line and the constraint. It means that the solution can be found by a direct method.

This algorithm has the advantage of being less costly than algorithm 1, but it has the disadvantage of choosing the interior point properly because the accuracy of the solution will depend strongly on the accuracy of this interior point. Figure 3 shows the behavior of the algorithm.

Algorithm 2
Given: $c \neq 0 \in \mathbb{R}^n$, $A \in R^{n\times n}$, symmetric and positive definite matrix and $b \in \mathbb{R}$, $b > 0$.

Step 1: Choose the starting point: $y_1 = 0$.

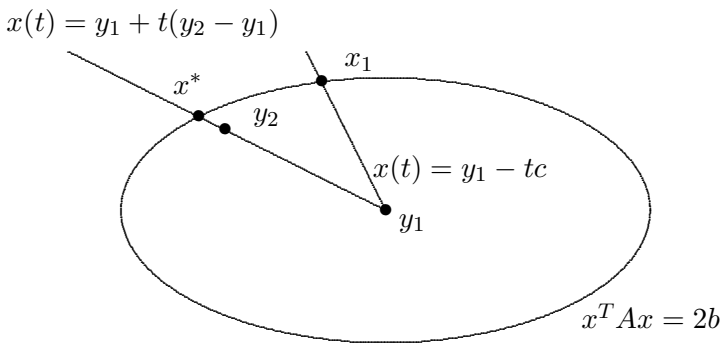

Figure 3: The behavior of the direct method

Step 2: Find a border point x_1 as the intersection between the halfline passing through y_1 in the direction $v = -c$ and the constraint.

Step 3: Find an interior point y_2 as the center of the resulting intersection between the level hyperplane $c^T x = c^T x_1$ and the constraint.

Step 4: Find the solution x^* as the intersection between the halfline passing through y_1 in the direction $v = y_2 - y_1$ and the constraint.

Let us analyze each step of the algorithm. There are no comments about **Step 1**, **Step 2** and **Step 3** because they are similar to those of **Algorithm 1**.

Let us consider **Step 4.** Since $y_1 = 0$, the point x^* is obtained as the intersection between the halfline $x(t) = ty_2,\ t > 0$, and the quadratic constraint $x^T Ax = 2b$. Then,

$$(ty_2)^T A(ty_2) = 2b, \quad t^* = \sqrt{\frac{2b}{y_2^T A y_2}}, \quad x^* = t^* y_2.$$

Then, **Algorithm 2** is established as

Algorithm 2:

Given: $c \neq 0 \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$ symmetric and positive definite$b \in \mathbb{R}$, $b > 0$.
Compute: B, e and $\widehat{A} = B^T AB$.

Step 1: Choose a starting interior point: $y_1 = 0$.

Step 2: Find a border point: $x_1 = -\sqrt{\frac{2b}{c^T Ac}}c$.

Step 3: Find an interior point: $y_2 = B\widehat{y}_2 + f_1 e$ with $\widehat{y}_2 = argmin\ \frac{1}{2}\widehat{x}^T \widehat{A}\widehat{x} - \widehat{d}^T\widehat{x}$,
where $f_1 = c^T x_1$ and $\widehat{d} = -f_1 B^T Ae$.

Step 4: Find the solution: $x^* = \sqrt{\frac{2b}{y_2^T A y_2}}y_2$.

6 Numerical experience

In this section implementations of Algorithms 1 and 2 are described. The algorithms have been implemented in Matlab in an environment PC with a Pentium 4 processor with 512 MB RAM

and 2.40GHz.

The specific procedure used is given below.

- The stopping criterion used in **Algorithm 1** is: $e_k = \|y_k - x_k\| < 10^{-12}$.
- In Step 1 of Algorithm 1 and Step 3 of Algorithm 2 the point $\widehat{y}_k = argmin\ \frac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d_k}^T\widehat{x}$ is obtained by applying the spectral gradient method. It is a relatively novel non-descent method, appropriate to large scale optimization problems and competitive with the traditional conjugate gradient method. For more details see [5, 7, 8, 9].

In the tables, the following abbreviations are used:

- **n**: the number of variable of the problem.
- **it**: the amount of iterations carried out by **Algorithm 1**.
- **Nit**: the number of iteration considered from **Algorithm 1**.
- **it SG**: the number of iterations required by spectral gradient method to obtain $\widehat{y}_k = argmin\ \frac{1}{2}\widehat{x}^T\widehat{A}\widehat{x} - \widehat{d_k}^T\widehat{x}$ in the k-th iteration.
- $f_k = c^T x_k$: the objective function value at the k-th iteration.
- $e_k = \dfrac{\|y_k - x_k\|}{\|x_k\|}$: the relative error in the k-th iteration.
- $f^* = c^T x^*$: the objective value function at the estimate x^*, given by the algorithm.
- $r = \|\frac{1}{2}{x^*}^T A x^* - b\|$: the error constraint evaluated at x^*. We observe that r should be zero since the solution must satisfy the constraint.
- **CPU time**: the computing time required by the algorithm.

Now, we consider two problems, each of them with different number of variables. Both problems are considered without the linear term ($d = 0$) because any other problem can be reduced to this case.

Problem 1:

Let us consider problem (4) with $c = (1, 1, ..., 1)^T \in \mathbb{R}^n$, $A = diagonal(1, 2, ..., n) \in \mathbb{R}^{n\times n}$ and $b = 1$.

Table 1 shows the results obtained at each iteration of the iterative method with $n = 100$. Tables 2 and 3 show the results obtained applying Algorithms 1 and 2 with different values of n (n =100, 200, 300, 400, 500, 600, 700, 800, 900 and 1000).

The fast convergence of the algorithm can be observed in Table 1: the error decreases quite fast. Also, it is possible to observe that the number of iterations required by the spectral gradient method to obtain y_k decreases as k increases.

Table 2 shows that the number of iterations required by Algorithm 1 do not increase when the number of variable is augmented. The time required to run the algorithm increases because of the operations needed at each iterations. Clearly, more computing time is needed if the number of variable is large.

Comparing Tables 2 and 3, there are not significant differences between the results obtained by Algorithms 1 and 2, despite the considerable decrease in computing time.

Nit	$f_k = c^T x_k$	$e_k = \frac{\|y_k - x_k\|}{\|x_k\|}$	**it SG**
1	-1.99007438041998	1	0
2	-2.96984668055811	0.18218129703840	132
3	-3.20683507409673	0.03193981609218	123
4	-3.22093665958930	0.00178265648084	111
5	-3.22098665492903	$6.297052951447885e-006$	94
6	-3.22098665555746	$7.915125095980291e-011$	76
7	-3.22098665555746	$5.035955884656709e-017$	18

Table 1: Iterations of Algorithm 1 - Problem 1, $n = 100$

n	$f^* = c^T x^*$	$r = \|\frac{1}{2} x^{*T} A x^* - b\|$	**CPU time**	**It**
100	-3.22098665555746	$3.330669073875470e-016$	0.0630	7
200	-3.42871140463044	$2.220446049250313e-016$	0.3430	7
300	-3.54476060695204	$3.330669073875470e-016$	1.4530	7
400	-3.62489439602770	$2.220446049250313e-015$	2.9850	7
500	-3.68587124842703	$9.992007221626409e-016$	5.9680	7
600	-3.73496410209512	$2.220446049250313e-015$	11.1250	7
700	-3.77597937377608	$1.332267629550188e-015$	18.9220	7
800	-3.81115527428657	$9.992007221626409e-016$	27.3750	7
900	-3.84191771929092	$1.110223024625157e-015$	38.9690	7
1000	-3.86923011994643	$2.220446049250313e-016$	56.9370	7

Table 2: Algorithm 1 applied to Problem 1 and different values of n

n	$f^* = c^T x^*$	$r = \|\frac{1}{2} x^{*T} A x^* - b\|$	**CPU time**
100	-3.22098665555746	$2.220446049250313e-016$	0.0320
200	-3.42871140463045	$8.881784197001252e-016$	0.1250
300	-3.54476060695204	$1.887379141862766e-015$	0.6400
400	-3.62489439602770	$8.881784197001252e-016$	1.4530
500	-3.68587124842704	$8.881784197001252e-016$	2.9850
600	-3.73496410209512	$1.332267629550188e-015$	5.3910
700	-3.77597937377609	$8.881784197001252e-016$	9.0470
800	-3.81115527428656	$5.551115123125783e-016$	12.5630
900	-3.84191771929092	$1.110223024625157e-016$	18.7970
1000	-3.86923011994643	$9.992007221626409e-016$	24.8750

Table 3: Algorithm 2 applied to Problem 1 and different values of n

Problem 2:

Let us consider problem (4) with $c = (1, 1, ..., 1)^T \in \mathbb{R}^n$, $b = 1$ and $A = \dfrac{H(v)^T H(v)}{n^3} \in \mathbb{R}^{n \times n}$, where $v = (1, 2, 3, ..., n) \in \mathbb{R}^n$ and $H(v)$ is a square Hankel matrix whose first column is v and whose elements are zero below the first anti-diagonal. This matrix is symmetric and positive definite.

Table 4 shows the results obtained at each iteration of the algorithm when $n = 100$. Tables

5 and 6 show the results obtained via Algorithms 1 and 2.

Nit	$f_k = c^T x_k$	$e_k = \frac{\|y_k - x_k\|}{\|x_k\|}$	**it SG**
1	-3.82499150774954	1	0
2	-7.25025696447532	0.09187993351090	875
3	-10.07701880238112	0.04035743849082	705
4	-12.17872638695642	0.02164347403184	753
5	-13.51681325907164	0.01141576228632	878
6	-14.16487459323087	0.00498514448544	695
7	-14.34312557007998	0.00130895964353	732
8	-14.35752222964941	$1.044190646555198e-004$	710
9	-14.35761670656568	$6.845619643013136e-007$	580
10	-14.35761671063453	$2.948193549052210e-011$	332
11	-14.35761671063453	0	27

Table 4: Iterations of Algorithm 1 - Problem 2, $n = 100$

n	$f^* = c^T x^*$	$r = \|\frac{1}{2} x^{*T} A x^* - b\|$	**CPU time**	**It**
100	-14.35761671063453	0	0.4060	11
200	-20.15598398495877	0	5.8910	13
300	-24.62326461541155	$1.110223024625157e-016$	25.4060	15
400	-28.39588023323513	0	78.4690	17
500	-31.72283979772807	$2.220446049250313e-016$	198.0780	18

Table 5: Algorithm 1 applied to Problem 2 and different values of n

n	$f^* = c^T x^*$	$r = \|\frac{1}{2} x^{*T} A x^* - b\|$	**CPU time**
100	-14.35761671063453	$2.220446049250313e-016$	0.0630
200	-20.15598398495877	0	0.7500
300	-24.62326461541155	$2.220446049250313e-016$	2.1880
400	-28.39588023323513	0	7.4060
500	-31.72283979772806	$2.220446049250313e-016$	13.3750

Table 6: Algorithm 2 applied to Problem 2 and different values of n

The observations done above are valid for Problem 2. However, it is possible to observe an increment in the number of iterations required by Algorithm 1 to achieve convergence. Moreover, it is possible to observe that the computing time required for running Problem 2 is higher than the one required for Problem 1. It is because in Problem 1, the matrix is sparse.

7 Conclusions

The problem of minimizing a linear function subject to a strictly convex quadratic constraint has been analyzed. The convergence of the algorithm is guaranteed via simple geometric considerations. The simplicity and the good behavior of proposed algorithm make it adequate to large

scale optimization problems. Since many topologic optimization problems are established as (1) the next objective is to extend the algorithm when the strictly convex quadratic constraints appear showing a block structure. The truss optimization problems, if many bars are involved, show this block structure and the extended algorithm might be successfully used.

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Thickness optimization of an elastic beam

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Abstract

An elastic beam of variable thickness subject to a vertical load is considered in this work. Finding the thickness distribution minimizing the compliance of the beam is the structural optimization problem to be solved. Different types of support conditions for the beam are also included in the analysis. The approach is based on the Haslinger and Mäkinen formulation, although the resulting optimization problem is solved in a different way. Finite elements method is used to obtain a suitable discretized problem. The optimization problem is solved by using interior point methods and trust-region strategies. Numerical results are reported.

Resumen

En este trabajo es considerada una viga de espesor variable sujeta a una carga vertical. El problema de optimización estructural a resolver consiste en hallar el espesor que minimiza la deformación de la viga. Se analiza el problema con diferentes tipos de condiciones de soporte en la viga. El trabajo está basado en la formulación propuesta por Haslinger y Mäkinen aunque el problema de optimización obtenido es resuelto con un método diferente. El método de elementos finitos es utilizado para formular el problema discreto. El problema de optimización es resuelto usando el método de puntos interiores y estrategias de región de confianza. Se muestran resultados numéricos.

Key words: nonlinear programming, structural optimization, finite element method.
Palabras Claves: programación no lineal, optimización estructural, método de elementos finitos.
AMS Subject Classification: 74P05, 65L60, 90C30, 90C51.

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1 Introduction

Our main objective in this work is to present an optimization model for solving a structural design problem. Particularly, we are interested in sizing optimization problems, where a typical size of a structure has to be optimized.

The model problem that we considered is well known in the structural optimization literature, however, the modelization technique presented here is simple because it avoids using complex tools and aspects from the sensitivity analysis. The sensitivity analysis is the usual theory for dealing this kind of problem (see [7, 12]). However, the computational aspects and numerical implementation based on it use to be sophisticated (see [1, 5, 8]).

We consider an elastic beam, of length l, subject to a vertical load f responding to the Euler-Bernoulli theory. This theory assumes that cross-sections perpendicular to the axis of the beam remain plane and perpendicular to the axis after deformation. Moreover, the transverse deflection w is given by the following fourth order differential equation

$$\frac{d^2}{dx^2}\left(b\frac{d^2w}{dx^2}\right) = q \quad \text{for} \quad 0 < x < l,$$

where $b = b(x)$ and $q = q(x)$ are given functions of variable x and w is the dependent variable.

Here, b is a function depending on material properties and on the shape of the cross-section area of the beam, q is the distributed load and w represents the transverse deflection. In addition to the differential equation, the deflection w has to satisfy suitable boundary conditions, given by the supporting conditions.

In our optimal design problem the variable e is the thickness of the beam (height of cross-section) and our goal is to find the thickness distribution that minimize the compliance of the beam or, equivalently, that maximize the stiffness of the beam. Under this condition, the cross-section is a function of the thickness, that is, $w = w(e)$.

For numerical experiments we consider a beam with variable thickness, represented by the interval $\Omega = [0, 1]$, and subject to different support conditions.

Though our approach of this problem, and part of its analysis, is based on the formulation of [6], the resulting optimization problem is solved in a different way.

Basically, our idea is to use the finite element method to obtain a suitable discretization of the continuous boundary value problem in order to formulate an optimization nonlinear problem subject to equality, inequality constraints and bounds on the variables. For numerical results we have used the code KNITRO ([15]), which is an implementation of interior point method in combination with trust-region strategies ([14]).

This work is organized as follows. In section 2 we present the thickness beam problem and give a first optimization formulation, in section 3 we develop the discretization of the continuous problem using the finite element method. In section 4 we describe the reformulated optimization problem derived from the discretization and in section 5 we give some numerical results. Finally, in section 6, we state some conclusions.

2 The problem

Let us consider an elastic beam fixed at both of its endpoints subject to a uniformly distributed vertical load $q(x)$ and variable thickness e. Under these assumptions, the deflection w is the solution of the following boundary value problem:

$$\frac{d^2}{dx^2}\left(\beta e(x)^3 \frac{d^2 w}{dx^2}\right) = q(x), \quad 0 < x < l, \tag{2.1}$$
$$w(0) = w(l) = \frac{dw}{dx}(0) = \frac{dw}{dx}(l) = 0,$$

where $\beta \in L^\infty([0,l])$ is a positive function depending on material properties and on the shape of the cross-section area of the beam.

The stiffness of the beam is characterized by the functional $J : H_0^2(\Omega) \to \mathbb{R}$ defined as

$$J(w(e)) = \int_0^l q(x)w(e)dx,$$

where $H_0^2(\Omega)$ represent the Sobolev space of functions whose second derivatives are square-integrable and satisfy the boundary conditions and $w(e)$ is the solution of the boundary value problem (2.1).

This functional, which represents the external energy of deformation, can be considered as a measure of flexibility of the beam. On the other hand, the decrease of this functional implies increasing of the stiffness, so the problem of maximizing the stiffness is equivalent to minimize the functional J. This functional frequently appears in structural optimization either in the objective function or in the constraint set of the problem ([2, 13]).

To formulate the mathematical problem, we add some conditions, besides (2.1), that the thickness e has to satisfy. This conditions define a set of admissible thicknesses C given by:

$$C = \left\{ \begin{array}{l} e \in C^{0,1}(\Omega) \,|\, 0 < e_{\min} \leq e \leq e_{max} \text{ in } \Omega, \\ |e(x_1) - e(x_2)| \leq \gamma |x_1 - x_2| \text{ for all } x_1, x_2 \in \Omega, \\ \int_0^l e(x)dx = \alpha, \quad \text{for some } \alpha > 0, \\ e \text{ is symmetrical in } \Omega \end{array} \right\},$$

i.e., C consists of functions that are uniformly bounded, uniformly Lipschitz continuous in $[0,l]$ and preserve the beam volume and due to the boundary conditions a symmetric property is required. All of such conditions make sense from the practical and physical point of view.

From numerical and implementation aspects we consider the set $\tilde{C}$ characterized by continuous and piecewise constant thickness functions. This last requirement implies to construct a stepped beam. Consequently, the optimization problem is given by

$$\text{Find } e^\star \in \tilde{C} \text{ such that}$$
$$w(e^\star) = \text{argmin } J(w(e)) = \text{argmin} \int_0^l q(x)w(e(x))dx$$
$$\text{where } w(e) \text{ satisfy the problem (2.1).}$$

To solve numerically this problem, we make a complete discretization of it, and we obtain a new problem defined by a finite number of design parameters.

3 Discretization of the State Problem

For a discretization of the continuous problem we use a finite element approach, that is, we discretize the domain Ω and write the weak formulation of the differential equation. See [11, 10].

Let $d \in \mathbb{N}$ be given and $\Delta h : 0 = a_0 < a_1 < \ldots < a_d = l$ be an equidistant partition of Ω with the step $h = l/d, a_i = ih$, $i = 0, \ldots, d$. Thus, we divide the interval Ω in d subintervals called elements. The $a_i, i = 0 \ldots, d$ are called nodes.

In order to obtain the weak formulation we consider an arbitrary element $\Omega_k = [a_k,\ a_{k+1}]$. Let V_h be a finite dimensional subspace of $H_0^2(\Omega)$, whose functions are continuous piecewise polynomials. Let $v \in V_h$ be an arbitrary test function.

Now, by using the standard integration-by-parts formula twice in Ω_k, we have

$$\int_{a_k}^{a_{k+1}} \left(\beta e^3 \frac{d^2v}{dx^2}\frac{d^2w}{dx^2} - vq\right) dx + \left[v\frac{d}{dx}\left(\beta e^3 \frac{d^2w}{dx^2}\right) - \frac{dv}{dx}\beta e^3 \frac{d^w}{dx^2}\right]_{a_k}^{a_{k+1}} = 0.$$

The variables at each node involve the deflection w and its derivative $\frac{dw}{dx}$.

In the case of a beam supporting a flexion, the terms which have to be evaluated at the endpoints, have structural interpretations ([10]). Thus, the natural boundary conditions involve specifications about the bending moment $\beta e^3 \frac{d^2w}{dx^2}$ and the shear force $\frac{d}{dx}\left(\beta e^3 \frac{d^2w}{dx^2}\right)$ at the endpoints.

For simplicity, we introduce the following notation

$$\begin{aligned} Q_1^k &= \left[\tfrac{d}{dx}\left(\beta e^3 \tfrac{d^2w}{dx^2}\right)\right]_{a_k}, & Q_2^k &= \left[\beta e^3 \tfrac{d^2w}{dx^2}\right]_{a_k}, \\ Q_3^k &= -\left[\tfrac{d}{dx}\left(\beta e^3 \tfrac{d^2w}{dx^2}\right)\right]_{a_{k+1}}, & Q_4^k &= -\left[\beta e^3 \tfrac{d^2w}{dx^2}\right]_{a_{k+1}}. \end{aligned}$$

Thus, the weak formulation is given by

$$\begin{aligned} 0 &= \int_{a_k}^{a_{k+1}} \left(\beta e^3 \frac{d^2v}{dx^2}\frac{d^2w}{dx^2} - vq\right) dx - v(a_k)Q_1^k \\ &\quad - \left(-\frac{dv}{dx}\right) Q_2^k - v(a_{k+1})Q_3^k - \left(-\frac{dv}{dx}\right) Q_4^k. \end{aligned} \tag{3.1}$$

See Fig. 1.

The variational formulation (3.1) requires that the interpolation functions to be twice continuously differentiable and has to satisfy interpolation conditions at the endpoints: $w(a_k),\ w(a_{k+1}),\ w'(a_k),\ u$ These four conditions imply that we need a cubic polynomial to interpolate $w(x)$ and we assign the nodal variables for the element Ω_k

$$\begin{aligned} u_1 &= w(a_k), & u_2 &= -w'(a_k) \\ u_3 &= w(a_{k+1}), & u_4 &= -w'(a_{k+1}). \end{aligned}$$

By using these nodal variables we have the following expression for w in Ω_k

$$\begin{aligned} w(x) &= u_1\phi_1(x) + u_2\phi_2(x) + u_3\phi_3(x) + u_4\phi_4(x) \\ &= \sum_{j=1}^{4} u_j\phi_j(x), \end{aligned} \tag{3.2}$$

where the functions ϕ_j are the cubic Hermitte polynomials.

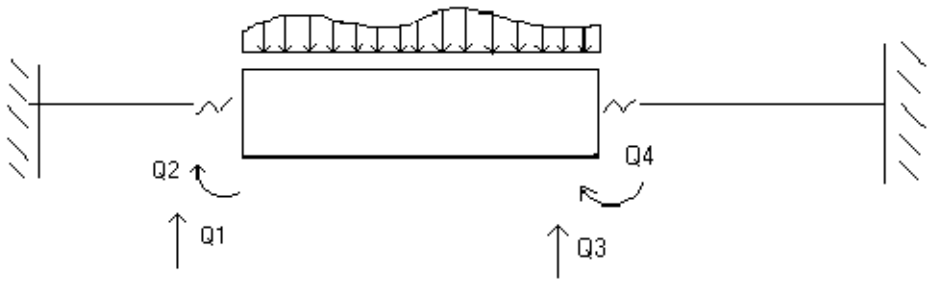

Figure 1: Generalized forces at one element of the beam.

3.1 The Finite Element Model

According to (3.2) and the interpolation functions ϕ_j in the weak formulation (3.1) we obtain the finite element model for the Euler-Bernoulli beam. Since there are four nodal variables at each element, then four possible choices could be used for v: $v = \phi_i, i = 1, \ldots, 4$.

For simplicity we consider the function β with constant value at the whole beam. Therefore, for the *i-th* algebraic equation (for $v = \phi_i$) we have that

$$\begin{aligned} 0 &= \beta e_k^3 \sum_{j=1}^{4} \left(\int_{a_k}^{a_{k+1}} \frac{d^2\phi_j^k}{dx^2} \frac{d^2\phi_i^k}{dx^2} dx \right) u_j \\ &\quad - \int_{a_k}^{a_{k+1}} \phi_i^k q(x) dx - Q_i^k, \end{aligned}$$

or equivalently,

$$\sum_{j=1}^{4} K_{ij}^k u_j^k - F_i^k = 0,$$

where

$$K_{ij}^k = \beta e_k^3 \int_{a_k}^{a_{k+1}} \frac{d^2\phi_j^k}{dx^2} \frac{d^2\phi_i^k}{dx^2} dx,$$

$$F_i^k = \int_{a_k}^{a_{k+1}} \phi_i^k q(x) dx + Q_i^k.$$

Now, if we write these coefficients in matrix notation we have

$$\begin{bmatrix} K_{11}^k & K_{12}^k & K_{13}^k & K_{14}^k \\ K_{21}^k & K_{22}^k & K_{23}^k & K_{24}^k \\ K_{31}^k & K_{32}^k & K_{33}^k & K_{34}^k \\ K_{41}^k & K_{42}^k & K_{43}^k & K_{44}^k \end{bmatrix} \begin{bmatrix} u_1^k \\ u_2^k \\ u_3^k \\ u_4^k \end{bmatrix} = \begin{bmatrix} q_1^k \\ q_2^k \\ q_3^k \\ q_4^k \end{bmatrix} + \begin{bmatrix} Q_1^k \\ Q_2^k \\ Q_3^k \\ Q_4^k \end{bmatrix},$$

where the matrix of the system, which is symmetric, is the stiffness matrix for the k-th element of the beam and the right hand side term is the vector of generalized forces, including the applied external forces and the shear force and flexion at the endpoints of the element.

If h is the length of the element and e is the thickness, the above equation is given by

$$K^k = \frac{2\beta e_k^3}{h^3}\begin{bmatrix} 6 & -3h & -6 & -3h \\ -3h & 2h^2 & 3h & h^2 \\ -6 & 3h & 6 & 3h \\ -3h & h^2 & 3h & 2h^2 \end{bmatrix},$$

$$F^k = \frac{qh}{12}\left\{\begin{bmatrix} 6 \\ -h \\ 6 \\ h \end{bmatrix} + \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{bmatrix}\right\}.$$

See [11].

3.2 Element Assembly

Having calculated the matrices and equations describing our approximations over each finite element, the next step is to assemble these equations on the entire mesh adding up the contributions furnished by each element. To do this, we take into account the two degrees of freedom at each node. That is, we consider the relationship between the variables associated to the right node at one particular element and the left node to the next element. In particular we consider the equilibrium relationships between the bending moment and the shear force between elements.

When the beam is partioned in d elements we obtain a $2(d+1)\times 2(d+1)$ assembly matrix. However, the algebraic system has $4(d+1)$ unknown variables, $2(d+1)$ correspond to the generalized forces vector and the other $2(d+1)$ to the deformations and its derivatives. Imposing the boundary conditions and the applied loads will allow us to reduce the unknown variables.

The boundary conditions for the beam problem depend on the geometric nature of the support conditions.

In the particular case of a beam fixed at both endpoints the deflection w and its derivative $\frac{dw}{dx}$ are zero at the endpoints. The equilibrium conditions, at the intermediate nodes, yield the equations

$$Q_3^k + Q_1^{k+1} = 0, \qquad Q_4^k + Q_2^{k+1} = 0,$$

because there are no forces applied there, whereas the shear force and the bending moment are unknown at the endpoints of the beam.

Now, by using the equilibrium conditions at the intermediate nodes we have the nonlinear system

$$K(e)U(e) = F(e),$$

where $K(e)$ is the stiffness matrix

$$\begin{bmatrix} 6e_1^3 & -3he_1^3 & \dots & 0 & 0 & 0 \\ -3he_1^3 & 2h^2e_1^3 & \dots & 0 & 0 & 0 \\ -6e_1^3 & 3he_1^3 & 6(e_1^3+e_2^3) & \dots & 0 & 0 \\ -3he_1^3 & h^2e_1^3 & 3h(e_1^3-e_2^3) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 3h(e_{d-1}^3-e_d^3) & -6e_d^3 & -3he_d^3 \\ 0 & \dots & \dots & 2h^2(e_d^3+e_{d-1}^3) & 3he_d^3 & h^2e_d^3 \\ 0 & \dots & \dots & 3he_d^3 & 6e_d^3 & 3he_d^3 \\ 0 & \dots & \dots & h^2e_d^3 & 3he_d^3 & 2h^2e_d^3 \end{bmatrix}$$

and

$$U(e) = \begin{bmatrix} 0 \\ 0 \\ u_3 \\ \vdots \\ \vdots \\ u_{2d} \\ 0 \\ 0 \end{bmatrix}, \qquad F(e) = \frac{qh^4}{24\beta} \left\{ \begin{bmatrix} 6 \\ -h \\ 12 \\ \vdots \\ \vdots \\ 6 \\ h \end{bmatrix} + \begin{bmatrix} Q_1^1 \\ Q_2^1 \\ 0 \\ \vdots \\ 0 \\ Q_3^d \\ Q_4^d \end{bmatrix} \right\}.$$

Since the equations that contain deflections and its slopes do not contain the unknown coefficients associated to the generalized forces, the corresponding equations can be solved independently. Thus, the matrix equation can be partitioned

$$\begin{bmatrix} K^{11} & K^{12} & K^{13} \\ K^{21} & K^{22} & K^{23} \\ K^{31} & K^{32} & K^{33} \end{bmatrix} \begin{bmatrix} U^1 \\ U^2 \\ U^3 \end{bmatrix} = \begin{bmatrix} F^1 \\ F^2 \\ F^3 \end{bmatrix},$$

where U^1 and U^3 contain the known deflection and derivatives (in this case are zero due the support conditions) and U^2 are the unknown. At the right hand side, in F^1 and F^3 there are unknown coefficients. Under this conditions the matrix equation that we are interested in, can be expressed as

$$K^{22}U^2 = F^2. \tag{3.3}$$

This is a $2(d-1) \times 2(d-1)$ system, whose unknown variables are the deflection and derivatives at the intermediate nodes of the discretization. The coefficients of the submatrix K^{22} depend on the thickness of each element of the beam.

4 Reformulation of the Optimization Problem

The discretization of the state problem yields a system of nonlinear algebraic equations (3.3). For the sake of simplicity of notation we rewrite the system (3.3) as

$$K(e)U(e) = F, \tag{4.1}$$

where $U(e)$ contains the deflection and its derivatives at the intermediate nodes. For the numerical solution of the problem we have to consider the conditions for the admissible thickness and discretization of the objective function.

The discretization of the state problem concern to the functional J, however, the restriction of J to the subspace V_h is identified with another functional defined in the euclidean space $\mathbb{R}^{2(d-1)}$ as in [6].

To do this, we discretize the integral by using the same numerical formula that we have used for the volume of the beam. Since we consider uniformly distributed load, that is $q(x) = q$, constant at the whole beam, and we also assume that the thickness is constant at each element it is enough to use the rectangle rule. Clearly, if the load were not uniformly distributed it would be better to use a higher order quadrature rule. Then, the objective function is approximated by

$$J(u(e)) = \int_0^l q(x)u(e(x))dx \simeq q^T \bar{U},$$

where $\bar{U}$ contains only the $d-1$ components of $U(e)$ associated to deflections at the intermediate nodes and q is a constant vector, which has the same size.

Since the discretized beam is stepped constant, the admissible thickness is defined by a piecewise constant function that satisfies the following conditions

$$e_{min} \leq e_i \leq e_{max}, \quad i = 1, \ldots, d,$$

$$\mid e_{i+1} - e_i \mid \leq \gamma h, \quad i = 1, \ldots, d-1,$$

for some constant γ. Moreover, the preserving volume condition is given by

$$h \sum_{i=1}^{i=d} e_i = \alpha.$$

Finally, the optimization problem is given by

$$\begin{aligned} \min_{e,U} \quad & q^T \bar{U} \\ \text{s.t.} \quad & K(e)U(e) = F \\ & h \sum_{i=1}^{i=d} e_i = \alpha, \\ & e_{min} \leq e_i \leq e_{max}, \quad i = 1, \ldots, d, \\ & \mid e_{i+1} - e_i \mid \leq \gamma h, \quad i = 1, \ldots, d-1. \end{aligned}$$

Thus, the above problem is the classical formulation of a nonlinear programming problem with bounds at the variables and equality and linear inequality constraints. It is worth noting that system of algebraic equations (4.1) is nonlinear strongly on the design variables e_i. Through the derivation of the model is similar to the presentation in [6], the formulation is conceptually different. In our approach the variables corresponding to thickness and deflection are related through the constraint equation $KU = F$, although initially they are independent. Moreover, in that presentation the optimization problem take into account the thicknesses and their relationship with the deflections trough a sensitivity analysis. While sensitivity analysis provides an elegant and mathematically rigorous method to formulate the problem, it has one very serious drawback: the numerical solution is very difficult to be computed.

5 Numerical Experiments

For numerical experiments we consider a beam with two different support conditions. First, we analyze a beam with both endpoints fixed, whose discretized model has been described in previous sections. Then, we consider a beam with one endpoint fixed and the other one simply supported. For this case, we note that the boundary conditions are different. At the simply supported endpoint the deflection is zero whereas its derivative is not: this support condition does not allow to assimilate bending moment at this endpoint. By using the notation of section 3, we have

$$w(0) = u_1^1 = 0; \ \left.\frac{dw}{dx}\right|_{x=0} = u_2^1 = 0;$$

$$w(l) = u_3^d = 0;\ Q_4^d = -\left[\beta e_d^3 \frac{d^2 w}{dx^2}\right]_l = 0.$$

According to these boundary conditions the nonlinear system of algebraic equations from the finite element method is modified.

For solving the optimization problem, we have used the solver KNITRO 3.1 ([14, 15]), by means of a Visual Fortran interface. The user has to provide three subroutines including the data of the problem, the objective function and the constraints, and finally, the gradient of the objective function and the Jacobian matrix of the constraints. This code is an implementation of the interior point method, where the nonlinear programming problem is solved by means of the solution of a sequence of barrier subproblems, depending on a parameter μ. On the other hand, the algorithm uses a trust-region method as a globalization strategy and a merit function to obtain global convergence results.

Each iteration of the subalgorithm generates steps whose normal and tangential components satisfy mild conditions on adequate models. The normal component improves the feasibility and the tangential component, which is computed using the projected conjugated gradient method, improves the optimality. The whole code KNITRO 3.1 computes some iterations for each subproblem before the barrier parameter is decreased and then the procedure is repeated until suitable convergence conditions are reached. See [4, 3] for a complete description and analysis of this method.

The number of elements used for numerical experiments in both problems was $d = 8$ and $d = 32$. For simplicity we adopted the following default values:

- $l = 1,$ the length of the beam.
- $\beta = 1; q(x) = -1$, the uniformly distributed load.
- $e_{\min} = 0.01$, $e_{\max} = 0.1$, bounds for the thickness.
- $\alpha = 0.05$, $\gamma = 0.5$.

The initial approximation for thickness were $e_i = 0.05, i = 1, \ldots, d$. Then we solved the linear system of algebraic equations (4.1) in order to obtain the initial values for the other variables.

Finally, we show in Fig. (2–3), the profile of the optimal solution for the beam problem, in both cases, and the corresponding optimal value of the objective function.

6 Conclusions

We have presented and tested an optimization formulation for the elastic beam problem, which is subject to vertical loads, as in Euler-Bernoulli theory.

One of the main advantage of this formulation is that it is possible to use any of the many available nonlinear programming method to solve the thickness problem. It is a very attractive feature due to the advances in optimization algorithm during the last years. On the other hand, researchers in engineering, applied mathematics and other sciences paid attention to the conexion between optimization and computational mechanics in structural problems (structural optimization), so important and interesting advances were done about this area recently.

Though we considered here a one dimensional model, the same ideas can be applied in more complicated structural problems of dimension 2 or 3, or subject to different support and loads.

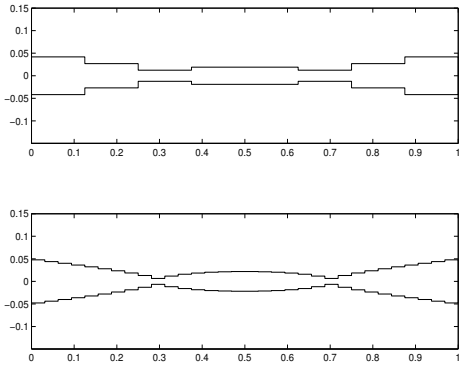

Figure 2: Discretization of the beam with both endpoints fixed by using 8 (J=6.388) and 32 elements (J=5.659) respectively.

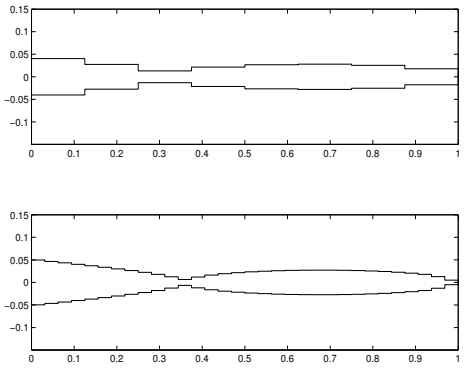

Figure 3: Discretization of the beam with endpoints fixed-simply supported by using 8 (J=29.458) and 32 elements (J=15.765) respectively.

The numerical results obtained are promising and encouraging. Moreover, the particular structure of the elastic beam problem obtained after the discretization seems to indicate that new optimization approach as Inexact–restoration methods ([9]) could be perform efficiently, particularly for large scale discretization.

In practice, it is usually important to optimize structures subject to different types of loads. In addition to the compliance cost functional we could consider another two functionals involving the smallest eigenvalues for two generalized problems. Eigenvalues represent natural frequencies of free oscillations and buckling loads of the beam and depend on the thickness distribution e. The goal could be to find a thickness minimizing the compliance of the perpendicularly loaded beam, maximizing the minimal natural frequency (i.e., the beam is stiffer under slowly varying dynamic forces), and maximizing the minimal buckling load (i.e., the beam does not loose its stability easily under the compressive load). So we would have a simple prototype of multiobjective thickness optimization of an elastic beam. It could be solved using nonlinear least squares if the solution of each problem is known. This will be the object of our practical research in the near future.

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Determinación de dos coeficientes térmicos a través de un problema de desublimación con acoplamiento de temperatura y humedad. *

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Resumen

Se considera un modelo de flujo de calor y humedad a través de un semiespacio poroso durante congelamiento, con sobrecondición de temperatura y de flujo de calor en el borde fijo para la determinación de dos coeficientes desconocidos del material semi-infinito de cambio de fase. Se trata de un problema de frontera móvil con acoplamiento de las funciones temperatura y concentración (ecuaciones de tipo Luikov) con ocho parámetros. Para dos de los casos de determinación posibles, se hallan condiciones necesarias y suficientes para la existencia de una solución y las fórmulas correspondientes para las temperaturas y concentraciones de ambas fases, como también para los coeficientes desconocidos.

Nomenclatura

a_m	difusividad de humedad
$c_i, i = 1, 2$	calor específico en la fase-i
$k_i,\ i = 1, 2$	conductividad térmica de la fase-i
q_0	coeficiente que caracteriza el flujo de calor en $x = 0$
r	calor latente
$s(t)$	posición del frente de evaporación
t	tiempo
$T_i,\ i = 1, 2$	temperatura en la fase-i.
t_0	temperatura inicial
t_s	temperatura en el borde fijo $x = 0$

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t_v	temperatura de cambio de fase $(t_s < t_v < t_0)$
u	potencial de transferencia de masa
u_0	potencial inicial de transferencia de masa
ρ	densidad de masa
δ	coeficiente de gradiente térmico
σ	constante que caracteriza la frontera móvil $s(t) = 2\sigma\sqrt{t}$
$\mathcal{L}u = \frac{\rho a_m c_2}{k_2}$	número de Luikov
$\mathcal{K}o = \frac{ru_o}{c_2(t_0-t_v)}$	número de Kossovitch
$\mathcal{P}n = \frac{\delta(t_0-t_v)}{u_o}$	número de Posnov

1. Introducción.

Los problemas de transferencia de calor y masa con cambio de fase que se llevan a cabo en un medio poroso, tales como evaporación, condensación, congelamiento, derretimiento, sublimación y desublimación, tienen una gran aplicación en procesos de separación, tecnología de alimentos, migración de calor en terrenos y suelos, etc. Debido a que este tipo de problemas es no lineal, el resolverlos usualmente tiene dificultades matemáticas. Sólo se han encontrado unas pocas soluciones exactas para casos ideales (ver [2],[3],[4] por ejemplo). Una extensa bibliografía sobre problemas de frontera libre y móvil para la ecuación de calor-difusión está dada en [12].

La formulación matemática de la transferencia de calor y masa en cuerpos de capilares porosos fue establecida por Luikov ([5],[6]). Mikhailov [7] presentó dos modelos diferentes para resolver el problema de la evaporación de humedad líquida desde un medio poroso. Para el problema del congelamiento (desublimación) de un semiespacio poroso húmedo, Mikhailov también presentó una solución exacta [8] para una condición de temperatura constante en el borde fijo $x = 0$. En el trabajo [9] fue presentada una solución explícita para las distribuciones de temperatura y humedad en un semiespacio poroso con una condición de flujo de calor en el borde fijo $x = 0$ del tipo $\frac{q_0}{\sqrt{t}}$.

Ahora se considerará el modelo presentado en [8]-[9] como un problema de frontera móvil, esto es $x = s(t)$ es conocida (dada por la expresión $s(t) = 2\sigma\sqrt{t}$ con $\sigma > 0$ una constante dada) con una sobrecondición en el borde fijo. Esto nos permite considerar dos coeficientes térmicos desconocidos y calcularlos bajo ciertas restricciones sobre los datos iniciales del problema siguiendo la idea de [13] para una fase y de [11] para dos fases.

Se considera el flujo de calor y humedad a través de un semiespacio poroso durante el congelamiento. La posición del frente de cambio de fase al tiempo t está dada por $x = s(t)$ que divide al cuerpo poroso en dos regiones. En la región congelada, $0 < x < s(t)$, no hay movimiento de humedad y la distribución de temperatura está descripta por la ecuación del calor

$$\frac{\partial T_1}{\partial t}(x,t) = a_1 \frac{\partial^2 T_1}{\partial x^2}(x,t), \qquad 0 < x < s(t),\ t > 0, \qquad a_1 = \frac{k_1}{\rho c_1}. \tag{1}$$

La región $s(t) < x < +\infty$ es la parte húmeda del cuerpo de capilares porosos en donde fluyen acoplados el calor y la humedad. El proceso está descripto por el ya conocido sistema de Luikov [6] para el caso $\varepsilon = 0$ (ε es el factor de conversión de fase de líquido en vapor) dado por

$$\frac{\partial T_2}{\partial t}(x,t) = a_2 \frac{\partial^2 T_2}{\partial x^2}(x,t), \qquad x > s(t),\ t > 0, \qquad a_2 = \frac{k_2}{\rho c_2} \tag{2}$$

$$\frac{\partial u}{\partial t}(x,t) = a_m \frac{\partial^2 u}{\partial x^2}(x,t), \qquad x > s(t),\ t > 0. \tag{3}$$

Las distribuciones iniciales de temperatura y humedad son uniformes

$$\begin{cases} T_2(x,0) = T_2(+\infty,t) = t_0, \\ u(x,0) = u(+\infty,t) = u_0. \end{cases} \tag{4}$$

Se supone que sobre la superficie del semiespacio la temperatura es constante

$$T_1(0,t) = t_s \tag{5}$$

donde $t_s < t_v$.

Sobre el frente de congelamiento, existe una igualdad entre las temperaturas

$$T_1(s(t),t) = T_2(s(t),t) = t_v, \qquad t > 0, \tag{6}$$

donde $t_v < t_0$.

El balance de calor y humedad en el frente de congelamiento da lo siguiente

$$k_1 \frac{\partial T_1}{\partial x}(s(t),t) - k_2 \frac{\partial T_2}{\partial x}(s(t),t) = \rho\, r\, u(s(t),t) \frac{ds}{dt}(t), \qquad t > 0, \tag{7}$$

$$\frac{\partial u}{\partial x}(s(t),t) + \delta \frac{\partial T_2}{\partial x}(s(t),t) = 0, \qquad t > 0. \tag{8}$$

Se considera además una sobre condición en el borde fijo $x = 0$ [1] considerando que el flujo de calor depende del tiempo de la siguiente manera

$$k_1 \frac{\partial T_1}{\partial x}(0,t) = \frac{q_0}{\sqrt{t}} \tag{9}$$

donde $q_0 > 0$ es un coeficiente que caracteriza el flujo de calor en el borde fijo $x = 0$.

En este trabajo, se considerará que la frontera móvil $x = s(t)$ definida para $t > 0$ con $s(0) = 0$, está dada por

$$s(t) = 2\sigma\sqrt{t} \tag{10}$$

donde $\sigma > 0$ es una constante dada (puede ser determinada por procesos experimentales).

El conjunto de ecuaciones y condiciones (1)-(10) será llamado problema P.

Se hallarán fórmulas para la determinación de dos coeficientes térmicos desconocidos elegido entre ρ (densidad de masa), a_m (difusividad de la humedad), c_1 (calor específico de la región congelada), c_2 (calor específico de la región húmeda), k_1 (conductividad térmica de la región congelada), k_2 (conductividad térmica de la región húmeda), δ (coeficiente de gradiente térmico), r (calor latente) junto con las temperaturas T_1, T_2 y la humedad u como función de los coeficientes térmicos y los datos t_0, t_s, t_v, q_0, u_0 y σ en dos de los veintiocho casos posibles.

Siguiendo [9], para el caso general $\mathcal{L}u = \frac{\rho a_m c_2}{k_2} \neq 1$ se tiene que

$$T_1(x,t) = t_v - \frac{\sqrt{\pi} q_0}{\sqrt{\rho c_1 k_1}} \left[-\operatorname{erf}\left(\gamma_0 \frac{x}{2\sqrt{t}}\right) + \operatorname{erf}(\gamma_0 \sigma) \right], \ 0 < x < s(t),\ t > 0 \tag{11}$$

$$T_2(x,t) = t_v + \frac{t_0 - t_v}{1 - \operatorname{erf}\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right)} \left[\operatorname{erf}\left(\sqrt{\frac{\mathcal{L}u}{a_m}} \frac{x}{2\sqrt{t}}\right) - \operatorname{erf}\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right) \right], \ x > s(t),\ t > 0 \tag{12}$$

$$u\left(x,t\right)=u_0-\gamma_1\left\{\text{erf}\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\frac{x}{2\sqrt{t}}\right)-\frac{\exp\left(\left(\frac{1}{\mathcal{L}u}-1\right)\frac{\mathcal{L}u}{a_m}\sigma^2\right)\left(1-\text{erf}\left(\frac{x}{2\sqrt{a_m t}}\right)\right)}{\sqrt{\mathcal{L}u}}\right\},\ x>s(t),\ t>0 \tag{13}$$

con

$$\gamma_0=\sqrt{\frac{\rho c_1}{k_1}},\quad \gamma_1=\frac{\delta\rho a_m c_2(t_0-t_v)}{k_2-\rho a_m c_2}=\frac{\mathcal{P}n}{\frac{1}{\mathcal{L}u}-1}, \tag{14}$$

donde los dos coeficientes térmicos desconocidos deben satisfacer el siguiente sistema de ecuaciones trascendentales:

$$\gamma_2\exp\left(-\left(\gamma_0\sigma\right)^2\right)-F_1\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right) = \gamma_3\sigma\left\{1-\gamma_1\left(1-\frac{Q(\frac{\sigma}{\sqrt{a_m}})}{Q\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right)}\right)\right\} \tag{15}$$

$$\text{erf}\left(\gamma_0\sigma\right) = \frac{1}{\gamma_4} \tag{16}$$

con

$$\gamma_2=\frac{\sqrt{\pi}q_0}{\sqrt{c_2k_2\rho}(t_0-t_v)},\quad \gamma_3=\sqrt{\frac{\pi\rho}{c_2k_2}}\frac{r\,u_0}{(t_0-t_v)}=\sqrt{\pi\frac{\mathcal{L}u}{a_m}}\mathcal{K}o,\quad \gamma_4=\frac{\sqrt{\pi}q_0}{\sqrt{c_1k_1\rho}(t_v-t_s)} \tag{17}$$

donde las funciones reales F_1 y Q están definidas por

$$F_1\left(x\right)=\frac{\exp\left(-x^2\right)}{\left(1-\text{erf}(x)\right)},\qquad Q\left(x\right)=\sqrt{\pi}x\exp\left(x^2\right)\left(1-\text{erf}(x)\right) \tag{18}$$

con las siguientes propiedades

$$F_1\left(0\right)=1,\qquad F_1\left(+\infty\right)=+\infty,\qquad F_1'\left(x\right)>0\quad\forall x>0 \tag{19}$$

$$Q\left(0\right)=0,\qquad Q\left(+\infty\right)=1,\qquad Q'\left(x\right)>0\quad\forall x>0. \tag{20}$$

De los 28 casos posibles en la presente comunicación sólo se considerará el caso de la determinación de los coeficientes térmicos $\{c_1,k_1\}$ y el de la determinación de los coeficientes térmicos $\{c_2,k_2\}$.

Teorema 1: (Determinación de los coeficientes térmicos $\{c_1,k_1\}$) Si

$$\gamma_5=\frac{1}{\gamma_2}\left\{F_1\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right)+\gamma_3\sigma(1-\gamma_1(1-\frac{Q(\frac{\sigma}{\sqrt{a_m}})}{Q\left(\sqrt{\frac{\mathcal{L}u}{a_m}}\sigma\right)}))\right\}<1 \tag{21}$$

con γ_1,γ_2 y γ_3 definidos en (14) y (17), y F_1 y Q definidas en (18) , entonces existe una única solución al problema P dada por (11)-(13), y los coeficientes térmicos k_1 y c_1 están dados por las siguientes expresiones

$$k_1=\frac{\sqrt{\pi}q_0}{(t_v-t_s)}F_2\left(\sqrt{\frac{1}{\log\left(\frac{1}{\gamma_5}\right)}}\right),\qquad c_1=\frac{\sqrt{\pi}q_0}{\sigma\rho(t_v-t_s)}M\left(\sqrt{\frac{1}{\log\left(\frac{1}{\gamma_5}\right)}}\right) \tag{22}$$

donde las funciones reales F_2 y M están definidas por

$$F_2\left(x\right)=\frac{\text{erf}\left(x\right)}{x},\qquad M\left(x\right)=x\,\text{erf}\left(x\right). \tag{23}$$

Demostración: Considerando $x = \sqrt{\frac{\rho c_1}{k_1}}\sigma$ e $y = \frac{\sqrt{\rho c_1 k_1}(t_v - t_s)}{\sqrt{\pi} q_0}$, el sistema (15)-(16) puede escribirse como

$$\exp\left(-x^2\right) = \gamma_5 \tag{24}$$

$$\operatorname{erf}(x) = y \tag{25}$$

De (24) surge trivialmente que $x = \sqrt{-\log(\gamma_5)}$. Notemos que $x > 0$ si y solamente si $0 < \gamma_5 < 1$. Teniendo en cuenta que γ_5 siempre es un número positivo, considerando el Lema 1 de [10] acerca del signo de $\frac{m^2-1}{1-\frac{Q(mx)}{Q(x)}}$, así que sólo se debe imponer que γ_5 debe ser menor que uno, i.e. la condición (21). Entonces, de (25) se tiene que $y = \operatorname{erf}\left(\sqrt{-\log(\gamma_5)}\right)$. Luego de algunos cálculos se obtiene (22).

Teorema 2: (Determinación de los coeficientes térmicos $\{c_2, k_2\}$) Si los datos verifican la condición

$$\frac{t_v - t_s}{\sigma r u_0}\sqrt{\frac{c_1 k_1}{\rho}}\frac{\exp\left(-(\gamma_0\sigma)^2\right)}{\operatorname{erf}(\gamma_0\sigma)} < 1 \tag{26}$$

entonces existen infinitas soluciones al problema P que vienen dadas por (11-13),

$$c_2 = \frac{k_2}{\sigma^2\rho}\xi^2 \tag{27}$$

donde ξ es una solución de la ecuación

$$P(x) = R(x), \ x > 0 \tag{28}$$

para cada $k_2 \in \mathbb{R}^+$, con

$$P(x) = 1 - \frac{a_m \mathcal{P}n \ x^2}{\sigma^2 - a_m x^2}\frac{Q(\frac{\sigma}{\sqrt{a_m}})}{Q(x)}, \qquad R(x) = \frac{q_0}{\sigma\rho r u_0}\exp\left[-(\gamma_0\sigma)^2\right] + \frac{k_2(t_0 - t_v)}{\sqrt{\pi}\sigma^2\rho r u_0} x F_1(x).$$

Demostración: Primero, los datos del problema deben verificar la condición (16). Luego, de (15) y considerando $x = \sqrt{\frac{\rho c_2}{k_2}}\sigma$ se tiene que

$$\frac{q_0}{\sigma\rho r u_0}\exp\left[-(\gamma_0\sigma)^2\right] + \frac{k_2(t_0 - t_v)}{\sqrt{\pi}\sigma^2\rho r u_0} x F_1(x) = 1 - \frac{a_m \mathcal{P}n x^2}{\sigma^2 - a_m x^2}\frac{Q(\frac{\sigma}{\sqrt{a_m}})}{Q(x)},$$

es decir, la ecuación (28). La función R tiene las siguientes propiedades:

$$R(0^+) = \frac{q_0}{\sigma\rho r u_0}\exp\left[-(\gamma_0\sigma)^2\right], \ R(+\infty) = -\infty, \ R'(x) < 0 \ \forall x > 0.$$

La función P tiene las siguientes propiedades:

$$P(0^+) = 1, \ P(+\infty) = 1 + \mathcal{P}n\left(1 - Q(\tfrac{\sigma}{\sqrt{a_m}})\right) > 1.$$

Por lo tanto, se tiene que ambas funciones se encontrarán en al menos un $x > 0$ si la condición $\frac{q_0}{\sigma\rho r u_0}\exp\left[-(\gamma_0\sigma)^2\right] > 1$ se verifica. Así, teniendo en cuenta (16), se halla una solución a la ecuación (28) si vale (26). Es sencillo ver que (27) surge de la definición de x. Este análisis puede hacerse para cualquier $k_2 > 0$ dado.

Los veintiseis casos restantes serán considerados en un futuro trabajo que se encuentra en etapa de preparación.

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MAT - Serie A, 14 (2007) 31-34

SOBRE LA NO CONVERGENCIA DEL MÉTODO DE MÍNIMOS CUADRADOS EN DIMENSIÓN INFINITA[§]

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Resumen. Un procedimiento muy utilizado en diversas aplicaciones para aproximar las soluciones de un problema inverso infinito-dimensional de la forma $Ax = b$, donde A es un operador lineal y compacto sobre un cierto espacio de Hilbert X y b es el dato dado, consiste en encontrar una sucesión $\{X_N\}$ de subespacios aproximantes finito-dimensionales de X cuya unión es densa en X y construir la sucesión $\{x_N\}$ de soluciones de mínimos cuadrados del problema en cada subespacio X_N. En [3], Seidman demostró que si el problema es mal condicionado, entonces sin ninguna hipótesis adicional sobre la solución exacta o sobre la sucesión de subespacios aproximantes $\{X_N\}$, no se puede garantizar que la sucesión $\{x_N\}$ convergerá a la solución exacta. En este artículo se extiende este resultado: se prueba que si X es separable, entonces para cualquier $b \in X$, $b \neq 0$, y para cualquier función no negativa definida sobre los naturales $f : \mathbb{N} \to \mathbb{R}^+$, existe un operador lineal, compacto e inyectivo A y una sucesión creciente de subespacios finito-dimensionales $X_N \subset X$ tales que $\|x_N - A^{-1}b\| \geq f(N)$ para todo $N \in \mathbb{N}$, donde x_N es la solución de mínimos cuadrados del problema $Ax = b$ en X_N.

1. Introducción y Preliminares

Dentro de un marco matemático bastante general un problema inverso lineal en dimensión infinita se puede presentar como la necesidad de determinar x en una ecuación de la forma

$$Ax = b, \tag{1.1}$$

donde $A : X \to Y$ es un operador lineal y acotado, X, Y son espacios de Hilbert de dimensión infinita, el rango de A no es cerrado y b es un dato conocido. En tal caso, la inversa generalizada de Moore-Penrose del operador A, $A^\dagger$, no es acotada y por lo tanto el problema inverso (1.1) es mal condicionado [1]. Es bien sabido que si $b \in \mathcal{R}(A^\dagger)$, la mejor solución aproximada (i.e. la solución de mínimos cuadrados de mínima norma) de (1.1) está dada por $x^\dagger \doteq A^\dagger b$. En lo que sigue nos referiremos a $x^\dagger$ como la "solución exacta" de (1.1). Un procedimiento estándar para aproximar las soluciones de este tipo de problemas es la estimación de mínimos cuadrados. Dada una sucesión creciente $\{X_N\}$ de subespacios de X de dimensión finita cuya unión es densa en X, x_N es solución de mínimos cuadrados en X_N si minimiza $\|Ax - b\|^2$ para $x \in X_N$.

Palabras clave. Mínimos Cuadrados, Espacios de Hilbert, inversa generalizada de Moore-Penrose.
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Es sabido que en problemas mal condicionados, sin supuestos adicionales sobre la solución exacta o sobre la sucesión de subespacios aproximantes X_N, no se puede garantizar que la sucesión de soluciones de mínimos cuadrados converja a la solución exacta. Más precisamente, T. Seidman probó en [3] que si X es un espacio de Hilbert separable de dimensión infinita, $B \doteq \{e_n\}_{n=1}^{\infty}$ es una base ortonormal de X y $X_N \doteq \text{span}\{e_1, ..., e_N\}$, entonces existen un operador lineal $A : X \to X$ compacto, inyectivo, autoadjunto y de rango denso en X y $b \in \mathcal{R}(A)$, $b = Ax^*$ para algún $x^* \in X$, tales que si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces $\|x_N - x^*\| \to \infty$. Es importante señalar aquí que esta falta de convergencia no es una consecuencia del método de mínimos cuadrados, sino de elegir la sucesión de subespacios aproximantes sin tener en cuenta el operador A que define el problema. Por ejemplo, Luecke y Hickey [2] probaron que cuando el operador A es compacto y los subespacios X_N son los autoespacios asociados a la descomposición en valores singulares de A, la sucesión de soluciones de mínimos cuadrados siempre converge a la solución exacta.

En este trabajo se extiende el resultado de Seidman en el siguiente sentido: se demuestra que es posible que la solución de mínimos cuadrados diverja de la solución exacta con cualquier velocidad arbitrariamente grande, prescrita a-priori. Para ello, necesitamos introducir las siguientes definiciones.

Definición 1.1. *Sean X un espacio de Hilbert separable de dimensión infinita y $B \doteq \{e_n\}_{n=1}^{\infty}$ una base ortogonal de X. Se dice que un elemento $x \in X$ es "degenerado con respecto a la base B" si puede escribirse como una combinación lineal finita de elementos de B; caso contrario se dice que x es "no degenerado con respecto a B". En particular, si $\langle x, e_n \rangle \neq 0 \ \forall \ n \in \mathbb{N}$ se dice que x es "fuertemente no degenerado con respecto a B". Si $\langle x, e_n \rangle \neq 0$ para infinitos valores de n, se dice que x es "débilmente no degenerado con respecto a B". Claramente, todo elemento fuertemente no degenerado en una base es también débilmente no degenerado en la misma base.*

2. Resultados Principales

El siguiente teorema afirma que dados un espacio de Hilbert separable de dimensión infinita arbitrario X y un elemento $b \in X$, $b \neq 0$, existe un operador lineal A tal que las soluciones de mínimos cuadrados del problema $Ax = b$ en X_N se alejan de la solución exacta con velocidad arbitrariamente grande. Por razones de brevedad presentaremos aquí sólo un bosquejo de la demostración. Mayores detalles pueden encontrarse en [4].

Teorema 2.1. ([4]) *Sean X un espacio de Hilbert separable de dimensión infinita y $f : \mathbb{N} \to \mathbb{R}^+$ una función creciente arbitraria. Entonces para cada $b \in X$, $b \neq 0$, existen una sucesión creciente de subespacios X_N cuya unión es densa en X y un operador lineal $A = A(b, f) : X \to X$, compacto, inyectivo y de rango denso en X, tales que $b = Ax^*$ para algún $x^* \in X$, y si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces $\|x_N - x^*\| \geqslant f(N)$ para todo $N \in \mathbb{N}$.*

Demostración. Dado $b \in X$, $b \neq 0$, es posible probar que existe una base ortonormal $B \doteq \{e_n\}_{n=1}^{\infty}$ de X tal que b es fuertemente no degenerado con respecto a B. Luego, dada esta base B, para cada par de sucesiones $\{\alpha_n\}$, $\{\beta_n\} \in \ell^2$ que satisfacen

$$\alpha_n \neq 0 \ \forall \ n \in \mathbb{N}, \ \beta_1 = 0, \ \beta_n \neq 0 \ \forall \ n \geq 2, \tag{2.1}$$

se tiene que el operador lineal $A : X \to X$ definido por

$$Ax \doteq \sum_{n=1}^{\infty} (\alpha_n \xi_n + \beta_n \xi_1)\, e_n,$$

donde $x = \sum_{n=1}^{\infty} \xi_n e_n \in X$, es compacto, inyectivo y tiene rango denso en X.

Por último, se puede ver que dado cualquier $b \in X$ fuertemente no degenerado con respecto a B es posible elegir las sucesiones $\{\alpha_n\}$, $\{\beta_n\} \in \ell^2$ de manera tal que, además de satisfacer (2.1), se tenga que $b \in \mathcal{R}(A)$ y, si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces $\|x_N - A^{-1}b\| \geq f(N)$ para todo $N \in \mathbb{N}$. □

Cuando se aplica el método de mínimos cuadrados para resolver problemas concretos, usualmente la base $B \doteq \{e_n\}_{n=1}^{\infty}$ está dada y los subespacios X_N se eligen como $X_N \doteq \text{span}\{e_1, ..., e_N\}$. En el siguiente resultado se muestra que en este caso, para cualquier $b \in X$ débilmente no degenerado con respecto a la base B y para cualquier función $f : \mathbb{N} \to \mathbb{R}^+$ creciente no negativa, es posible construir un operador $A = A(b, f)$ tal que las soluciones de mínimos cuadrados de $Ax = b$ en X_N diverjan de la solución exacta con velocidad arbitraria. Nuevamente presentamos aquí sólo un bosquejo de la demostración de este resultado.

Corolario 2.2. ([4]) *Sean X un espacio de Hilbert separable de dimensión infinita, $f : \mathbb{N} \to \mathbb{R}^+$ una función creciente arbitraria, $B \doteq \{e_n\}_{n=1}^{\infty}$ una base ortonormal de X, $b \in X$ débilmente no degenerado con respecto a la base B y $X_N \doteq \text{span}\{e_1, ..., e_N\}$. Entonces existe un operador lineal $A = A(b, f) : X \to X$, compacto, inyectivo y de rango denso en X tal que $b = A\hat{x}$ para algún $\hat{x} \in X$ y, si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces $\|x_N - \hat{x}\| \geqslant f(N)$ para todo $N \in \mathbb{N}$.*

Demostración. Se definen

$$\Delta \doteq \{n \in \mathbb{N} : \langle b, e_n \rangle \neq 0\}, \quad \Gamma \doteq \mathbb{N} \setminus \Delta,$$

$$B^{\Delta} \doteq \{e_{n_j} : n_j \in \Delta\}, \quad B^{\Gamma} \doteq \{e_{m_j} : m_j \in \Gamma\}$$

y $X_b \doteq \overline{\text{span}\, B^{\Delta}}$. Es inmediato que

$$\overline{\text{span}\, B^{\Gamma}} = X_b^{\perp}$$

y que b es fuertemente no degenerado con respecto a la base B^{Δ} de X_b. Como X_b es un espacio de Hilbert separable de dimensión infinita, el Teorema 2.1 implica que existe un operador lineal $A^{\Delta} : X_b \to X_b$ compacto, inyectivo y de rango denso en X_b tal que $b = A^{\Delta}\hat{x}$ para algún $\hat{x} \in X_b$ y si x_M^{Δ} es la solución de mínimos cuadrados de $A^{\Delta}x = b$ en

$$X_M^{\Delta} \doteq \text{span}\, \{e_{n_j}\}_{j=1}^{M} \subset X_b,$$

entonces

$$\left\|x_M^{\Delta} - \hat{x}\right\| \geq \tilde{f}(M) \; \forall \; M \in \mathbb{N},$$

donde $\tilde{f}(j) \doteq f(n_{j+1})$.

Finalmente, se construye el operador A como una extensión apropiada de A^{Δ} a todo el espacio X. La forma en que se realiza esta extensión depende de la cardinalidad del conjunto Γ. □

Puede pensarse que el resultado del corolario anterior tiene poca relevancia desde el punto de vista práctico pues podría suceder que en un entorno de b, el único valor de $\eta \in \mathcal{R}(A)$ para el cual se tiene que las soluciones de mínimos cuadrados de $Ax = \eta$ en X_N satisfacen que $\|x_N - A^{-1}\eta\| \geqslant f(N)$ para todo $N \in \mathbb{N}$ sea, precisamente, $\eta = b$. Sin embargo, en el siguiente resultado se prueba que esto no es así. En efecto, veremos que en todo entorno reducido de centro en b y radio $\delta > 0$ existe una sucesión $\{b_k^{\delta}\}_{k=1}^{\infty} \subset \mathcal{R}(A)$ tal que $b_k^{\delta} \to b$ cuando $k \to \infty$ y $\left\|x_N^k - A^{-1}b_k^{\delta}\right\| \geqslant f(N)$ para todo $N \in \mathbb{N}$, donde x_N^k es la solución de mínimos cuadrados de $Ax = b_k^{\delta}$ en X_N. Es decir, para cada elemento de la sucesión $\{b_k^{\delta}\}_{k=1}^{\infty}$ (i.e. para cada k fijo), las soluciones de mínimos cuadrados aproximantes

$\{x_N^k\}_{N=1}^{\infty}$, también se alejan de la solución exacta con velocidad arbitrariamente grande, de la misma forma con que lo hacen las soluciones de mínimos cuadrados obtenidas con dato igual a b.

Corolario 2.3. *Sean X un espacio de Hilbert separable de dimensión infinita, $B \doteq \{e_n\}_{n=1}^{\infty}$ una base ortonormal de X, $X_N \doteq \text{span}\{e_1, ..., e_N\}$, $f : \mathbb{N} \to \mathbb{R}^+$ una función creciente arbitraria, $b \in X$ no degenerado con respecto a B y $A = A(b, f)$ el operador cuya existencia se probó en el Corolario 2.2. Entonces, en todo entorno reducido de centro en b y radio $\delta > 0$ existe una sucesión $\{b_k^\delta\}_{k=1}^{\infty} \subset \mathcal{R}(A)$ tal que $b_k^\delta \to b$ cuando $k \to \infty$ y para cada $k \in \mathbb{N}$, la solución de mínimos cuadrados x_N^k de $Ax = b_k^\delta$ en X_N verifica que $\left\|x_N^k - A^{-1}b_k^\delta\right\| \geqslant f(N)$ para todo $N \in \mathbb{N}$.*

Demostración. Sea $\delta > 0$ dado, definimos $b_k^\delta \doteq \left(1 + \frac{\delta}{2k\|b\|}\right) b$ para cada $k \in \mathbb{N}$ ($b \neq 0$ por ser no degenerado con respecto a β). Como $0 < \left\|b_k^\delta - b\right\| = \frac{\delta}{2k} < \delta$, se tiene que $\{b_k^\delta\}_{k=1}^{\infty}$ está en el entorno reducido de centro en b y radio δ. Claramente, $b_k^\delta \to b$ cuando $k \to \infty$. Puesto que $\mathcal{R}(A)$ es un subespacio de X, resulta que $b_k^\delta \in \mathcal{R}(A) \,\forall\, k \in \mathbb{N}$. Si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces $x_N^k \doteq \left(1 + \frac{\delta}{2k\|b\|}\right) x_N$ es la solución de mínimos cuadrados de $Ax = b_k^\delta$ en X_N. Ahora bien,

$$\begin{aligned} \left\|x_N^k - A^{-1}b_k^\delta\right\| &= \left(1 + \frac{\delta}{2k\,\|b\|}\right) \left\|x_N - A^{-1}b\right\| \\ &\geq \left\|x_N - A^{-1}b\right\| \\ &\geq f(N) \,\forall\, N \in \mathbb{N}, \end{aligned}$$

donde la última desigualdad se sigue del Corolario 2.2.

□

Obs. 1. *En la demostración se usó el siguiente resultado: si x_N es la solución de mínimos cuadrados de $Ax = b$ en X_N, entonces σx_N con $\sigma \neq 0$, es la solución de mínimos cuadrados de $Ax = \sigma b$ en X_N.*

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MAT - Serie A, 14 (2007), 35-40

AN ALTERNATIVE METHOD TO COMPUTE MICHAELIS-MENTEN PARAMETERS FROM NUTRIENT UPTAKE DATA

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Abstract. An alternative method to compute the Michaelis-Menten parameters for nutrient uptake kinetics is presented. The method uses the explicit integration in time of the differential equation obtained from the relationship between decreasing nutrient concentration in a given volume of solution culture and nutrient uptake by roots. Thus, the depletion curve C = C(t) is obtained. Then, by using a non linear least squares fit method we obtain good estimations of the initial first derivative (rate of nutrient uptake) and the initial second derivative of the concentration. With these values and the average concentration at large times, explicit formulas for J_m (maximum influx at infinity concentrations), K_M (the Michaelis-Menten constant) and E (the efflux) are obtained. The method is applied to the pioneer depletion curve obtained by Claassen and Barber. Results obtained by Claassen-Barber, linearization Hanes method, non linear fit method applied to C´(t) vs. C and our method are compared. The results shown that the error obtained by our method is significantly smaller for the parameter E in contrast to the results obtained by the other methods.

Key words: Depletion curves, solution culture, kinetic parameters.

Introduction

One of the methods of generating nutrient uptake data is the pioneer nutrient depletion method of Claassen and Barber (1974). By this method, growing plants absorbing nutrient in a limited volume of nutrient solution decrease the nutrient concentrations over a short period of time. Aliquots are removed and analyzed for concentrations of the nutrient of interest. In a simple case, volume changes due to evapotranspiration and quantities of nutrients withdrawn with the aliquots are small to the point of being negligible. The slope of concentration with respect to time is the rate of nutrient uptake, i.e. dC/dt, and the rate of nutrient uptake can be measured for a range of concentrations in a single experiment as the nutrient concentration is drawn down by plant uptake.

By assuming Michelis-Menten kinetics (Michaelis-Menten, 1913) with an additional term of efflux rate E, the rate of absorption of nutrient can be described by the differential equation

$$\frac{dC(t)}{dt} = -\frac{\ell}{V}\left[\frac{J_m C}{K_M + C} - E\right] \qquad (1)$$

where C is the concentration of nutrient in soil solution, ℓ is root length, V is the volume of nutrient solution, J_m is the influx a infinity concentrations, K_M is the Michaelis-Menten constant and E is a constant efflux rate. This equation is generally applicable to this situation and the issue divides in two problems: to express Michaelis-Menten kinetics in an integral form as a function of time or to make a parameter optimization of the coefficients J_m and K_m in order to generate the best fit of the kinetic model to the experimental data. For the first case the Michaelis-Menten equations can be analytically integrated in order to give an explicit expression in C but not in t. This means that if C is measured, then with values of E, J_m, K_M,

and C_o, the time t predicted by the Michaelis-Menten kinetics model to drawn down concentrations to that value of C could be calculated. Alternatively, the Michaelis-Menten differential equation can be numerically integrated by Euler or Runge-Kutta's methods. Another methods used are the Hanes linearization (Hanes, 1932) method and the non linear least squares fit method applied to C´(t) vs. C (Levemberg, 1944; Marquardt, 1963) which are widely applied in biochemical sciences to estimate parameters of Michaelis-Menten kinetics.

Our method

In order to solve the first case we consider the differential problem for the depletion curve (Claassen and Barber, 1974), which is given by:

$$\frac{dC(t)}{dt} = -A\left[\frac{J_m C}{K_M + C} - E\right] \quad , \quad C(0) = C_o \tag{2}$$

with $A = \dfrac{\ell}{V}$. By integration of the Cauchy differential problem (2) we obtain:

$$\nu t = G\left(\frac{(J_m - E)C(t) - EK_M}{(J_m - E)C_o - EK_M}\right) = G\left[1 + \frac{(J_m - E)\big(C(t) - C_o\big)}{(J_m - E)C_o - EK_M}\right] = G\big[1 - \eta\big(C_o - C(t)\big)\big] \tag{3}$$

where:

$$\nu = \frac{\big(J_m - E\big)^2 A}{\big(J_m - E\big)C_o - EK_M}, \quad \eta = \frac{J_m - E}{\big(J_m - E\big)C_o - EK_M} \tag{4}$$

and real function G is defined by:

$$\begin{aligned} &G(x) = 1 - x - \mu \log x, \qquad 0 < x < 1, \\ &\mu = \frac{K_M J_m}{\big(J_m - E\big)C_o - EK_M} \end{aligned} \tag{5}$$

By using the following properties

$$G(0^+) = +\infty, \quad G(1) = 0, \quad G'(x) < 0, \quad 0 < x < 1 \tag{6}$$

and the real inverse function $F(x) = G^{-1}(x)$, defined for x > 0, which satisfies the properties

$$F(0^+) = 1, \quad F(+\infty) = 0, \quad F'(x) < 0, \quad \forall x > 0 \tag{7}$$

then we get the following explicit expression for the concentration C(t) versus time t:

$$C(t) = \frac{EJ_m}{J_m - E} + \left(C_o - \frac{EK_M}{J_m - E}\right) F(\nu t), \ t > 0 \tag{8}$$

Now, from the depletion curve C = C(t), are obtained the following experimental data:

$$\begin{aligned} &C'(0) = -\alpha, \qquad \alpha > 0 \\ &C''(0) = \beta \\ &C(\infty) = \gamma \end{aligned} \tag{9}$$

These data are related with the efflux E, the maximum influx at infinity concentrations J_m and the Michaelis-Menten K_M constant through the following analytical relations obtained from the expression for C(t) shown above, i.e.:

$$\begin{aligned} & A\left[\frac{J_m C_o}{C_o + K_M} - E\right] = \alpha \\ & \frac{A^2 K_M J_m}{\left(C_o + K_M\right)^3}\left[\left(J_m - E\right)C_o - EK_M\right] = \beta \\ & \frac{EK_M}{J_m - E} = \gamma \end{aligned} \tag{10}$$

Solving the system of three equations for the unknown E, J_m, K_M we obtain the following expressions for E, J_m and K_M.

$$\begin{aligned} E &= \frac{\alpha}{A\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right) - 1\right]} \\ J_m &= \frac{\gamma\beta}{A\alpha}\frac{\left(\frac{C_o}{\gamma} - 1\right)^2}{\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right) - 1\right]\left[1 - \frac{\beta\gamma}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right)\right]} \\ K_M &= \gamma\frac{\left[\frac{\beta C_o}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right) - 1\right]}{\left[1 - \frac{\beta\gamma}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right)\right]} \end{aligned} \tag{11}$$

Moreover, from the above formulas obtained for E, J_m and K_M as functions of the coefficients α, β and γ we deduce that a necessary and sufficient condition in order to have positive E, J_m and K_M parameters is given by the following inequalities:

$$\frac{\gamma}{C_o} < \frac{\gamma\beta}{\alpha^2}\left(\frac{C_o}{\gamma} - 1\right) < 1 \tag{12}$$

From this, we remark that coefficients α, β and γ are not independent. The independent dimensionless coefficients are:

$$\xi = \frac{C_o}{\gamma} > 1 \text{ and } \eta = \frac{\alpha^2}{\beta\gamma} > 0 \tag{13}$$

which determine the admissible region given by:

$$\xi - 1 < \eta < \xi(\xi - 1) \tag{14}$$

Previously to apply our method, in order to obtain a more exact results is necessary a very good estimation of $C'(0) = -\alpha$ and $C''(0) = \beta$. By using (3) we transform the expression (8) in an equivalent expression:

$$C(t) = C_o - \frac{1}{\eta} I(\nu t) \tag{15}$$

where $I:[0,+\infty) \to [0,1)$ is the inverse function of the $H:[0,1) \to [0,+\infty)$ defined by the expression

$$H(x) = x - \mu \log(1-x) \tag{16}$$

which has the following properties

$$H'(x) = 1 + \frac{\mu}{1-x} > 0, \quad H''(x) = \frac{\mu}{(1-x)^2} > 0, \quad H'''(x) = \frac{2\mu}{(1-x)^3}, \quad 0 \le x < 1$$

$$H(0^+) = 0, \quad H(1^-) = +\infty, \qquad H'(0^+) = 1+\mu, \quad H''(0^+) = \mu, \quad H'''(0) = 2\mu \tag{17}$$

Moreover, function I(x) has the following properties:

$$I(0^+) = 0, \quad I(+\infty) = 1, \qquad I'(0^+) = \frac{1}{1+\mu}, \quad I''(0^+) = -\frac{\mu}{(1+\mu)^3}, \quad I'''(0^+) = \frac{\mu(\mu-2)}{(1+\mu)^5}$$

Now, in order to fit the depletion curve C(t) vs. t we define a new function

$$\Gamma(t) = 1 - \frac{C(t)}{C_o} = \frac{1}{C_o \eta} I(\nu t) \cong \frac{1}{C_o}\left[P_1 t - P_2 t^2 + P_3 t^3\right] \tag{18}$$

where:

$$P_1 = \frac{\nu}{\eta(1+\mu)}, \quad P_2 = \frac{\mu\nu^2}{2\eta(1+\mu)^3}, \quad P_3 = \frac{\mu(2-\mu)\nu^3}{6\eta(1+\mu)^5} \tag{19}$$

The coefficients P_1, P_2, and P_3 are obtained from fitted curve $\Gamma(t)$ versus t. Then, the coefficients ν, η, and μ can be obtained analytically solving the system of three equations (19) which solution is given by:

$$\nu = \frac{9}{2}\frac{\left(P_1P_3 + 2P_2^2\right)^2}{P_1P_2\left(3P_1P_3 + 2P_2^2\right)}, \quad \eta = \frac{3}{2}\frac{P_1P_3 + 2P_2^2}{P_1^2P_2}, \quad \mu = \frac{4}{3}\frac{P_2^2}{3P_1P_3 + 2P_2^2} \tag{20}$$

and therefore the coefficients α and β are given by:

$$\alpha = \frac{\nu}{\eta(1+\mu)} = P_1, \quad \beta = \frac{\mu\nu^2}{\eta(1+\mu)^3} = 2P_2 \tag{21}$$

The coefficient γ is obtained by averaging the last four values of C(t).

Results and Discussion

By using the experimental data for concentrations (mol cm^{-3}) from Claassen-Barber, 1974: y_o = 0.1918 x 10^{-6}, y_1 = 0.1713 x 10^{-6}, y_2 = 0.1509 x 10^{-6}, y_3 = 0.1266 x 10^{-6}, h = 600 sec., solution volume = 2800 cm^3, root length = 28610 cm (Claassen, N. 2000, personal communication) and

taking for large time the arithmetic mean of the last four values of the depletion curve of Claassen-Barber, we obtain 22.81 pmoles cm^{-1} s^{-1} for J_m, 576.6 mmoles cm^{-3} for K_M y 0.1299 pmoles cm^{-1} s^{-1} for E. In Table I we show a comparison between the different results obtained by Claassen-Barber method, linearization method of Hanes, non linear fit method applied to C´(t) vs. C and our method.

Table 1. J_m, K_M, E parameters computed by Claassen-Barber, Hanes, Non linear least squares methods and our method as described in this paper

Parameter	*Claassen-Barber method* §	*Hanes method*		*Non linear least squares fit of C'(t) vs. C method*#		*Our method*	
			% Error		% Error		% Error
J_m (pmoles cm^{-1} s^{-1})	4	10.54	21.1	11.7	3	22.81	16.7
K_M (mmoles cm^3)	27.9	180	19.5	11.5	17.2	576.6	33.8
E (pmoles cm^{-1} s^{-1})	0.18	0.274	61	0.143	156	0.1299	24.16
k (x 10^{-4} s^{-1}) *	0.143	0.586	40.6	1.02	20.2	0.4019	50.5

§ Data obtained from Claassen-Barber paper
# Results obtained applying the non linear fit (Levemberg-Marquadt) of the software Microcal Origin 7.5
*As defined by Cushman $k = J_m/K_M$ (Cushman, 1979)

As it can be appreciated, the non linear least squares method gives us the best value for J_m and K_M parameters. Instead, our method predicts the best value for E. Moreover, in Figure 1 we show the different curves C(t) vs. t obtained by integrating the equation (1) with the results obtained by the four methods.

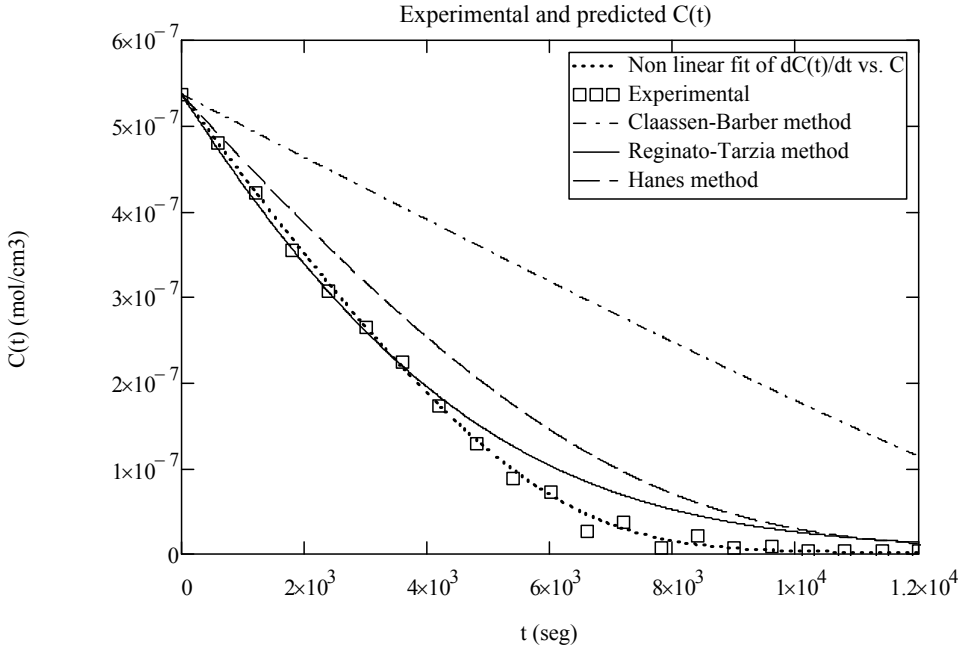

Figure 1. A comparison of the curves C(t) vs. t obtained by the four methods. Integration was performed with the mathematical package Mathcad

From the comparison between the experimental and predicted curves C(t) we observe that the best prediction is provided by the non linear least squares method and our method produces the second best prediction.

We have presented an alternative method to compute the Michaelis-Menten parameters of kinetics of nutrient uptake. The simplicity of the method is given by the utilization of few data (a good determination of initial first and second derivative, and the value of concentration at large times obtained from an explicit depletion curve) and the computation of J_m (maximum influx at infinity concentrations), K_M (the Michaelis-Menten constant) and E (the efflux) through explicit formulas. With respect to experimental data we obtain reasonable values for J_m and K_M although with greater errors than those obtained by the non linear least squares method. In the case of the efflux E we obtain a more exact result with respect to Hanes and non linear least squares methods. This last fact shows that the election of method to determine kinetic parameters not only depends of type de equations which parameters we desire to know but in addition of the algorithm used. The present method have been applied in the determination of kinetic parameters for potassium uptake by maize roots (Dekalb 762) growing in a typical Hapludol soil from Rio Cuarto, Cordoba. The results obtained were applied to validate a moving boundary model of nutrient uptake (Reginato et. al, 1999) and a model of coupled kinetics absorption of P and N by maize (Bernardo, 2005).

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MAT

INDICE GENERAL

Serie A: CONFERENCIAS, SEMINARIOS Y TRABAJOS DE MATEMÁTICA

ISSN 1515-4904

- Adriana B. Verdiell – María C. Maciel – Susana L. Orofino – Tatiana I. Gibelli, “A survey of the spectral gradient method”, 1-14.
- María F. Natale – Domingo A. Tarzia, “An integral equation in order to solve a one-phase Stefan problem with nonlinear thermal conductivity”, 15-24.
- María C. Sanziel – Domingo A. Tarzia, “Optimization on the heat flux in a mixed elliptic problem with temperature constraints”, 25-30.
- Claudia M. Gariboldi – Domingo A. Tarzia, “A new proof of the convergence of distributed optimal controls on the internal energy in mixed elliptic problems”, 31-42.

8 (2004): Domingo A. Tarzia (Ed.), “Primeras Jornadas sobre Ecuaciones Diferenciales, Optimización y Análisis Numérico”, Segunda Parte:

- Rubén D. Spies, “Differentiability of the solutions of a semilinear abstract Cauchy problem with respect to parameters”, 1-10.
- Adriana C. Briozzo – María F. Natale – Domingo A. Tarzia, “An explicit solution for a two-phase Stefan problem with a similarity exponencial heat sources”, 11-19.
- Domingo A. Tarzia, “An explicit solution for a two-phase unidimensional Stefan problem with a convective boundary condition at the fixed face”, 21-27.

9 (2005): Micol Amar – Roberto Gianni, “A Brief Survey on Homogenization with a Physical Application”.

10 (2005): Domingo A. Tarzia – Cristina V. Turner (Eds.), “Segundas Jornadas sobre Ecuaciones Diferenciales, Optimización y Análisis Numérico”:

- Marcos Gaudiano – Cristina Turner, “Difusión de un solvente en un polímero vidrioso con una condición de contorno del tipo creciente en el tiempo”, 1-9.
- Adriana C. Briozzo – María F. Natale – Domingo A. Tarzia, “A one-phase Lamé-Clapeyron-Stefan problem with nonlinear thermal coefficients”, 11-16.
- Eduardo A. Santillan Marcus - Domingo A. Tarzia, “Un caso de determinación de coeficientes térmicos desconocidos de un material semiinfinito poroso a través de un problema de desublimación con acoplamiento de temperatura y humedad”, 17-22.

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- María C. Maciel – Elvio A. Pilotta – Graciela N. Sottosanto, “Thickness optimization of an elastic beam”, 13-23.
- María F. Natale – Eduardo A. Santillan Marcus – Domingo A. Tarzia, “Determinación de dos coeficientes térmicos a través de un problema de desublimación con acoplamiento de temperatura y humedad”, 25-30.
- Rubén D. Spies – Karina G. Temperini, “Sobre la no convergencia del método de mínimos cuadrados en dimension infinita”, 31-34.
- Juan C. Reginato – Domingo A. Tarzia, “An alternative method to compute Michaelis-Menten parameters from nutrient uptake data”, 35-40.

Serie B: CURSOS Y SEMINARIOS PARA EDUCACIÓN MATEMÁTICA

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