A Fictitious Time Integration Method (FTIM) for Solving Mixed Complementarity Problems with Applications to Non-Linear Optimization

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Abstract: In this paper we propose a novel method for solving a nonlinear optimization problem (NOP) under multiple equality and inequality constraints. The Kuhn-Tucker optimality conditions are used to transform the NOP into a mixed complementarity problem (MCP). With the aid of (nonlinear complementarity problem) NCP-functions a set of nonlinear algebraic equations is obtained. Then we develop a fictitious time integration method to solve these nonlinear equations. Several numerical examples of optimization problems, the inverse Cauchy problems and plasticity equations are used to demonstrate that the FTIM is highly efficient to calculate the NOPs and MCPs. The present method has some advantages of easy numerical implementation, ease of treating NOPs, and the ease of extension to higher-dimensional NOPs.

Keyword: Nonlinear optimization problem, Mixed complementarity problem, NCP-functions, Fictitious time integration method (FTIM)

1 Introduction

In this paper we consider the following nonlinear optimization problem, subject to equality and inequality constraints:

$$\min f(\mathbf{x}),\tag{1}$$

$$\mathbf{h}(\mathbf{x}) = \mathbf{0},\tag{2}$$

$$\mathbf{g}(\mathbf{x}) \ge \mathbf{0},\tag{3}$$

where $f: \mathbb{R}^n \to \mathbb{R}$, $\mathbf{h}: \mathbb{R}^n \to \mathbb{R}^{m_1}$, and $\mathbf{g}: \mathbb{R}^n \to \mathbb{R}^{m_2}$ are differentiable functions.

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The extremal problem has had a long development history. After the works of Newton and Lebnitz on differential calculus, Fermat derived a necessary condition for obtaining the extremum of a single-variable function. For the extremal problem with equality constraints, Lagrange derived his famous Lagrange multipliers method in 1760. As for the extremal problem with inequality constraints, it is Kuhn and Tucker (1951) who gave a general condition which is necessary for optimality.

Nowadays, one of the Kuhn-Tucker conditions is well known for its complementary trios' structure. Equations including the complementary trios appear in many engineering problems, and they are called complementarity problems. A general complementarity problem is to find a solution $\mathbf{x} \in \mathbb{R}^n$ of the following complementary trios system:

$$\mathbf{P}(\mathbf{x}) \ge \mathbf{0}, \ \mathbf{Q}(\mathbf{x}) \ge \mathbf{0}, \ \mathbf{P}^{\mathrm{T}}\mathbf{Q} = 0, \tag{4}$$

where $\mathbf{P}, \mathbf{Q} \in \mathbb{R}^n$ denote vector functions. Many applications from engineering sciences, economics, game theory, etc. lead to problems of this kind; see Ferris and Pang (1997) for a survey. Most algorithms for the solution of nonlinear complementarity problem (NCP) are based on a suitable reformulation either as a system of algebraic equations, as an optimization problem, or as a fixed-point problem, etc. We refer the reader to the survey paper by Harker and Pang (1990) for the basic ideas of some algorithms. In fact, many of these reformulations can be obtained for a more general mixed complementarity problem (MCP), which includes complementary trios and algebraic equations [Dirkse and Ferris (1995a, 1995b); Kanzow (2001)].

The new method in this paper is based on a reformulation of the complementarity problem (4) as a system of nonlinear algebraic equations (NAEs):

$$\mathbf{F}(\mathbf{x}) = \mathbf{0},\tag{5}$$

where $\mathbf{F} \in \mathbb{R}^n$ is defined componentwise by

$$F_i(\mathbf{x}) := \phi(P_i(\mathbf{x}), Q_i(\mathbf{x})) \tag{6}$$

for some mapping $\phi:\mathbb{R}^2\mapsto\mathbb{R}$ having the property of

$$\phi(a,b) = 0 \Leftrightarrow a \ge 0, \ b \ge 0, \ ab = 0. \tag{7}$$

Clearly, this property guarantees that a vector $\mathbf{x} \in \mathbb{R}^n$ is a solution of the complementarity problem (4) if and only if \mathbf{x} solves the equations system (5). Applying Newton's method to system (5) then leads to one class of semismooth methods; see

Chen, Chen and Kanzow (2000), De Luca, Facchinei and Kanzow (1996, 2000), Facchinei and Kanzow (1997), Jiang, Fukushima, Qi and Sun (1998), Jiang and Qi (1997), Ulbrich (2001), Yamashita and Fukushima (1997), Ito and Kunisch (2007), and Chen and Pan (2008a) for some references. Depending on the choice of the mapping ϕ , different methods with different properties can be obtained. Some of these methods have been discussed in detail by Kanzow (2004).

Most semismooth methods have a very strong theoretical background and seem to be quite reliable and efficient also from a numerical point of view, at least when an exact Newton-type method is applied to system (5). However, in the large-scale case, we may not be able to find the exact solution of the corresponding linearized equation. There are other methods to solve the NCPs, such as smoothing or nonsmoothing Newton method [Qi and Sun (1993); Taji and Miyamoto (2002)], and homotopy method [Watson (1979)]. Usually, the resulting NAEs from the equivalent formulation of NCP-function are non-smooth, highly nonlinear as well as implicit, and it is desired to develop more efficient methods to obtain the solutions. In addition to the above NCP-functions method, there are penalty-function and barrier-function methods, which are used to transform the optimization problems into the solutions of algebraic equations; see the monograph by Bazaraa, Sherali and Shetty (1993), and references therein. The present approach of solving a nonlinear optimization problem is new and effective, and due to its easy implementation it may be useful in many engineering optimization problems, such as the rapidly growing field of topology optimization of mechanical structures [Wang and Wang (2004), Wang and Wang (2006), Wang, Lim, Khoo and Wang (2007a, 2007b, 2007c, 2008), Li and Atluri (2008a, 2008b)].

2 A fictitious time integration method

2.1 Kuhn-Tucker conditions

For the nonlinear optimization problem in Eqs. (1)-(3), the necessary conditions for \mathbf{x} to be a minimal point are the Kuhn-Tucker conditions:

$$\nabla f(\mathbf{x}) + \sum_{i=1}^{m_1} \mu_i \nabla h_i(\mathbf{x}) - \sum_{i=1}^{m_2} \lambda_i \nabla g_i(\mathbf{x}) = \mathbf{0},$$
(8)

$$h_i(\mathbf{x}) = 0, \quad i = 1, \dots, m_1, \tag{9}$$

$$\lambda_i \ge 0, \ g_i(\mathbf{x}) \ge 0, \ \lambda_i g_i = 0, \ i = 1, \dots, m_2.$$
 (10)

Both μ_i and λ_i are called the Lagrange multipliers.

For later convenience we call

$$L = f(\mathbf{x}) + \sum_{i=1}^{m_1} \mu_i h_i(\mathbf{x}) - \sum_{i=1}^{m_2} \lambda_i g_i(\mathbf{x})$$
(11)

a Lagrangian function, and hence Eq. (8) is written as $\nabla L = 0$.

Under a constraint qualification, which means that ∇g_i for $i = 1, ..., m_2$ belong to the active constraints and ∇h_i for $i = 1, ..., m_1$ are linearly independent, the Kuhn-Tucker conditions are necessary conditions, which also provide a way of finding optimal solutions.

2.2 Transformation of NCP into an algebraic equations system

The NCP in Eq. (10) under some conditions can be transformed into a mathematically equivalent problem, posed by algebraic equations and optimization equations. Let x be a solution of an NCP, that is, $x \ge 0$, $F(x) \ge 0$, and xF(x) = 0. Obviously, it is equivalent to the requirement that x is a solution of the minimum problem: $\min(x, F(x)) = 0$. The function ϕ is said to be an NCP-function: if $\phi : \mathbb{R}^2 \mapsto \mathbb{R}$ and $\phi(a,b) = 0$ iff $a \ge 0$, $b \ge 0$, ab = 0.

In addition to the minimum function, there are many other NCP-functions: for example, the Fischer-Burmeister [Fischer (1992)] NCP-function:

$$\phi_{\text{FB}}(a,b) = \sqrt{a^2 + b^2} - (a+b). \tag{12}$$

Thus for a general NCP of Eq. (4), we write it to be

$$F_i = \phi_{FB}(P_i, Q_i) = \sqrt{P_i^2 + Q_i^2} - (P_i + Q_i) = 0, \quad i = 1, \dots, n,$$
(13)

where P_i and Q_i are respectively the components of **P** and **Q**.

Up to now one of the most powerful approaches that has been studied intensively is to reformulate the NCP as a system of NAEs [Mangasarian (1976); Yamashita and Fukushima (1997)], or as an unconstrained minimization problem [Mangasarian and Solodov (1993); Yamashita and Fukushima (1995); Chen, Gao and Pan (2008)]. A function that can constitute an equivalent unconstrained minimization problem for the NCP is called a merit function. In other words, a merit function is a function whose global minima are coincident with the solutions of the original NCP. For constructing a merit function, the class of NCP-functions serves an important role. Some more in-depth studies of the NCP-functions and merit functions can be found in Facchinei and Soares (1997), Sun and Qi (1999), Chen (2006, 2007), and Chen and Pan (2008b).

2.3 Transformation of an algebraic equation into an ODE

We consider a single nonlinear algebraic equation:

$$F(x) = 0. (14)$$

In the above equation, we only have an independent variable x. We transform it into a first-order ordinary differential equation (ODE) by introducing a time-like or fictitious variable t into the following transformation of variables from x to y:

$$y(t) = (1+t)x.$$
 (15)

Here, t is a variable which is independent of x; hence, $\dot{y} = dy/dt = x$. If $v \neq 0$, Eq. (14) is equivalent to

$$0 = -\nu F(x). \tag{16}$$

Adding the equation $\dot{y} = x$ to Eq. (16) we obtain:

$$\dot{y} = x - vF(x). \tag{17}$$

By using Eq. (15) we can derive

$$\dot{y} = \frac{y}{1+t} - vF\left(\frac{y}{1+t}\right). \tag{18}$$

This is a first-order ODE for y(t). The initial condition for the above equation is y(0) = x, which is however an unknown and requires a guess.

Multiplying Eq. (18) by an integrating factor of 1/(1+t) we can obtain

$$\frac{d}{dt}\left(\frac{y}{1+t}\right) = -\frac{v}{1+t}F\left(\frac{y}{1+t}\right). \tag{19}$$

Further using y/(1+t) = x, leads to

$$\dot{x} = -\frac{v}{1+t}F(x). \tag{20}$$

The above idea is first proposed by Liu (2008a) to treat an inverse Sturm-Liouville problem by transforming an ODE into a PDE. Then, Liu (2008b, 2008c) and Liu, Chang, Chang and Chen (2008) extended this idea to develop new methods for estimating parameters in the inverse vibration problems. Recently, Liu and Atluri (2008) have employed the above technique of fictitious time integration method (FTIM) to solve large system of NAEs, and showed that high performance can be achieved by using the FTIM. Furthermore, Liu (2008d, 2008e) has used the FTIM technique to solve the NCPs and boundary value problems of elliptic PDEs, whose numerical results found to be excellent.

2.4 Transforming into a system of ODEs

First we apply the NCP-function in Eq. (12) to Eq. (10) and obtain

$$\sqrt{\lambda_i^2 + g_i^2} - (\lambda_i + g_i) = 0, \quad i = 1, \dots, m_2.$$
(21)

Eqs. (8), (9) and (21) constitute $N = n + m_1 + m_2$ nonlinear algebraic equations for the N unknowns of x_i , i = 1, ..., n, μ_i , $i = 1, ..., m_1$ and λ_i , $i = 1, ..., m_2$.

Then we use Eq. (20) in each equation to derive the following ODEs:

$$\dot{x}_i = \frac{-v_1}{1+t} \left[\frac{\partial f}{\partial x_i} + \sum_{j=1}^{m_1} \mu_j \frac{\partial h_j}{\partial x_i} - \sum_{j=1}^{m_2} \lambda_j \frac{\partial g_j}{\partial x_i} \right], \tag{22}$$

$$\dot{\mu}_i = \frac{-\nu_2}{1+t} h_i,\tag{23}$$

$$\dot{\lambda}_i = \frac{-v_3}{1+t} \left[\sqrt{\lambda_i^2 + g_i^2} - (\lambda_i + g_i) \right]. \tag{24}$$

The above equations can be written as vector forms, and the coefficients v_i , i = 1,2,3, more generally, can be the diagonal matrice with different values on the diagonal. Many numerical methods can be used to solve the above ODEs; however, a more stable one allowing large step length is described below for the Group-Preserving Scheme (GPS) developed previously by Liu (2001).

2.5 Group-preserving scheme for the system of ODEs

We can write Eqs. (22)-(24) as

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}, t), \ \mathbf{y} \in \mathbb{R}^N,$$
 (25)

where
$$\mathbf{y} = (x_1, ..., x_n, \mu_1, ..., \mu_{m_1}, \lambda_1, ..., \lambda_{m_2})^{\mathrm{T}}$$
.

A group-preserving scheme (GPS) can preserve the internal symmetry group of the considered ODEs system. Although we do not know previously the symmetry group of differential equations system, Liu (2001) has embedded it into an augmented differential equations system, which concerns with not only the evolution of state variables themselves but also the evolution of the magnitude of the state variables vector. Let us note that

$$\|\mathbf{y}\| = \sqrt{\mathbf{y}^{\mathsf{T}}\mathbf{y}} = \sqrt{\mathbf{y} \cdot \mathbf{y}},\tag{26}$$

where the dot between two N-dimensional vectors denotes their inner product. Taking the derivatives of both the sides of Eq. (26) with respect to t, we have

$$\frac{d\|\mathbf{y}\|}{dt} = \frac{\dot{\mathbf{y}}^{\mathrm{T}}\mathbf{y}}{\sqrt{\mathbf{y}^{\mathrm{T}}\mathbf{y}}}.$$
 (27)

Then, by using Eqs. (25) and (26) we can derive

$$\frac{d\|\mathbf{y}\|}{dt} = \frac{\mathbf{f}^{\mathsf{T}}\mathbf{y}}{\|\mathbf{y}\|}.\tag{28}$$

It is interesting that Eqs. (25) and (28) can be combined together into a simple matrix equation:

$$\frac{d}{dt} \begin{bmatrix} \mathbf{y} \\ \|\mathbf{y}\| \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{N \times N} & \frac{\mathbf{f}(\mathbf{y}, t)}{\|\mathbf{y}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{y}, t)}{\|\mathbf{y}\|} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \|\mathbf{y}\| \end{bmatrix}.$$
 (29)

It is obvious that the first row in Eq. (29) is the same as the original equation (25), but the inclusion of the second row in Eq. (29) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X} := (\mathbf{y}^T, \|\mathbf{y}\|)^T$, which satisfies the cone condition:

$$\mathbf{X}^{\mathsf{T}}\mathbf{g}\mathbf{X} = 0,\tag{30}$$

where

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_N & \mathbf{0}_{N \times 1} \\ \mathbf{0}_{1 \times N} & -1 \end{bmatrix}$$
 (31)

is a Minkowski metric, and I_N is the identity matrix of order N. In terms of (y, ||y||), Eq. (30) becomes

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X} = \mathbf{y} \cdot \mathbf{y} - \|\mathbf{y}\|^{2} = \|\mathbf{y}\|^{2} - \|\mathbf{y}\|^{2} = 0.$$
(32)

It follows from the definition given in Eq. (26), and thus Eq. (30) is a natural result. Consequently, we have an N+1-dimensional augmented system:

$$\dot{\mathbf{X}} = \mathbf{A}\mathbf{X} \tag{33}$$

with a constraint (30), where

$$\mathbf{A} := \begin{bmatrix} \mathbf{0}_{N \times N} & \frac{\mathbf{f}(\mathbf{y},t)}{\|\mathbf{y}\|} \\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{y},t)}{\|\mathbf{y}\|} & 0 \end{bmatrix}, \tag{34}$$

satisfying

$$\mathbf{A}^{\mathrm{T}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0},\tag{35}$$

is a Lie algebra so(N,1) of the proper orthochronous Lorentz group $SO_o(N,1)$. This fact prompts us to devise the group-preserving scheme (GPS), whose discretized mapping G must exactly preserve the following properties:

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G} = \mathbf{g},\tag{36}$$

$$\det \mathbf{G} = 1, \tag{37}$$

$$G_0^0 > 0,$$
 (38)

where G_0^0 is the 00-th component of **G**.

Although the dimension of the new system is raised by one more, it has been shown that the new system permits a GPS given as follows [Liu (2001)]:

$$\mathbf{X}_{k+1} = \mathbf{G}(k)\mathbf{X}_k,\tag{39}$$

where \mathbf{X}_k denotes the numerical value of \mathbf{X} at t_k , and $\mathbf{G}(k) \in SO_o(N,1)$ is the group value of \mathbf{G} at t_k . If $\mathbf{G}(k)$ satisfies the properties in Eqs. (36)-(38), then \mathbf{X}_k satisfies the cone condition in Eq. (30).

The Lie group can be generated from $\mathbf{A} \in so(N,1)$ by an exponential mapping,

$$\mathbf{G}(k) = \exp[h\mathbf{A}(k)] = \begin{bmatrix} \mathbf{I}_N + \frac{(a_k - 1)}{\|\mathbf{f}_k\|^2} \mathbf{f}_k \mathbf{f}_k^{\mathsf{T}} & \frac{b_k \mathbf{f}_k}{\|\mathbf{f}_k\|} \\ \frac{b_k \mathbf{f}_k^{\mathsf{T}}}{\|\mathbf{f}_k\|} & a_k \end{bmatrix}, \tag{40}$$

where

$$a_k := \cosh\left(\frac{h\|\mathbf{f}_k\|}{\|\mathbf{y}_k\|}\right),\tag{41}$$

$$b_k := \sinh\left(\frac{h\|\mathbf{f}_k\|}{\|\mathbf{y}_k\|}\right). \tag{42}$$

Substituting Eq. (40) for G(k) into Eq. (39), we obtain

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \eta_k \mathbf{f}_k,\tag{43}$$

$$\|\mathbf{y}_{k+1}\| = a_k \|\mathbf{y}_k\| + \frac{b_k}{\|\mathbf{f}_k\|} \mathbf{f}_k \cdot \mathbf{y}_k,$$
 (44)

where

$$\eta_k := \frac{b_k \|\mathbf{y}_k\| \|\mathbf{f}_k\| + (a_k - 1)\mathbf{f}_k \cdot \mathbf{y}_k}{\|\mathbf{f}_k\|^2}.$$
(45)

This scheme preserves the group properties for all h > 0, and is called the group-preserving scheme.

2.6 Numerical procedure

Starting from an initial value of $\mathbf{y}(0)$, we employ the above GPS to integrate Eq. (25) from t = 0 to a selected final time t_f . In the numerical integration process we can check the convergence of y_i at the k- and k + 1-steps by

$$\sum_{i=1}^{N} (y_i^{k+1} - y_i^k)^2 \le \varepsilon_1^2, \tag{46}$$

where ε_1 is a selected criterion. If at a time $t_0 \le t_f$ the above criterion is satisfied, then the solution of y_i is obtained. In practice, if a suitable t_f is selected, we find that the numerical solution also approach very well the true solution, even when the above convergent criterion is not satisfied. The coefficients v_1 , v_2 and v_3 introduced in Eqs. (22)-(24) can increase the stability of numerical integration.

In particular we may also use the following convergence criterion:

$$|f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k)| \le \varepsilon_2. \tag{47}$$

The present method is a new fictitious time integration method (FTIM), which can calculate the solution very stably and effectively. Below we give numerical examples to display some advantages of the present FTIM. Both convergence criteria will be used case by case; when we use criterion (46) the value of ε_1 will be written, and when we use criterion (47) the value of ε_2 will be written.

3 Numerical tests

3.1 Example 1

We first treat a very simple optimization problem:

$$\min x^2,
x \ge 1,$$
(48)

which is however used to demonstrate the technique of FTIM. The Lagrangian is

$$L = x^2 - \lambda(x - 1). \tag{49}$$

By using the Kuhn-Tucker conditions and the NCP of minimum we come to

$$2x - \lambda = 0,$$

$$\lambda \ge 0, \ x - 1 \ge 0, \ \lambda(x - 1) = 0 \Leftrightarrow \min(\lambda, x - 1) = 0.$$
(50)

It is simple to derive that $(x, \lambda) = (1, 2)$ is the optimal solution.

However, the FTIM leads to the following ODEs:

$$\dot{x} = \frac{-V_1}{1+t}(2x-\lambda),$$

$$\dot{\lambda} = \frac{-V_2}{1+t}\min(\lambda, x-1).$$
(51)

We apply the FTIM on this problem by starting from the initial conditions of x=2 and $\lambda=0.5$. Under the following parameters: h=1, $v_1=10$, $v_2=20$ and $\varepsilon_1=10^{-7}$, the convergence is very fast within 142 steps, and through very little computational time, about 0.1 second, the results are given by x=1.00000005 and $\lambda=2.0000014$. The path of (x,λ) is shown in Fig. 1.

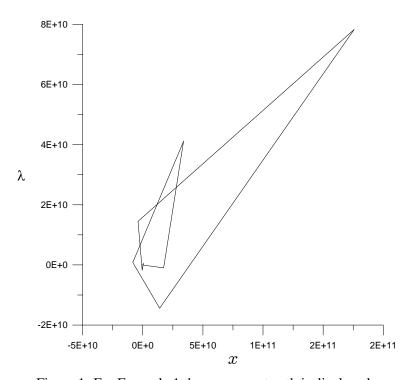


Figure 1: For Example 1 the convergent path is displayed.

3.2 Example 2

Then we treat another optimization problem:

$$\min 100(x_2 - x_1^2)^2 + (1 - x_1)^2,$$

$$x_1, x_2 \ge 0.$$
(52)

Kuo, Chang and Liu (2006) have used the particle swarm method to solve this problem; however, the numerical procedures are rather complex.

For this problem the resulting ODEs by the FTIM are

$$\dot{x}_{1} = \frac{-v_{1}}{1+t} \left[-400x_{1}(x_{2} - x_{1}^{2}) - 2(1-x_{1}) - \lambda_{1} \right],
\dot{x}_{2} = \frac{-v_{2}}{1+t} \left[200(x_{2} - x_{1}^{2}) - \lambda_{2} \right],
\dot{\lambda}_{1} = \frac{-v_{3}}{1+t} \left[\sqrt{\lambda_{1}^{2} + x_{1}^{2}} - \lambda_{1} - x_{1} \right],
\dot{\lambda}_{2} = \frac{-v_{3}}{1+t} \left[\sqrt{\lambda_{2}^{2} + x_{2}^{2}} - \lambda_{2} - x_{2} \right].$$
(53)

Here the exact minimal value is zero at $x_1 = x_2 = 1$.

We apply the FTIM on this problem by starting from the initial conditions of $x_1 =$ 0.8, $x_2 = 0.95$ and $\lambda_1 = \lambda_2 = 0.01$ and with the following parameters: h = 0.01, $v_1 = 0.1$, $v_2 = -0.05$, $v_3 = 30$ and $\varepsilon_2 = 10^{-6}$. The convergence is very fast within eight steps, and through a very little computational time, the results are given by $x_1 = 1.004484, x_2 = 1.009142, \lambda_1 = 0.05964447$ and $\lambda_2 = 0.05967688$. The computed minimal value is 2.24677×10^{-5} , whose accuracy is up to the fifth order.

Next we start from the initial conditions of $x_1 = 1.9$, $x_2 = 2$ and $\lambda_1 = \lambda_2 = 1$ and with the following parameters: h = 0.001, $v_1 = 1$, $v_2 = 10$, $v_3 = -100$ and $\varepsilon_2 = 10$ 10^{-10} . The minimal result is given by 3.5038×10^{-6} , whose accuracy is up to the sixth order. This example demonstrates that the FTIM is insensitive to the guesses of initial conditions.

3.3 Example 3

Wächter and Biegler (1999) have considered the following optimization problem:

$$\min x_1,
x_1^2 - x_2 + a = 0,
x_1 - x_3 - b = 0,
x_2, x_3 \ge 0.$$
(54)

They showed that under some conditions the sequence of points generated by interior-point algorithm remain bounded away from the optimum value. It is easy to see that x_2 and x_3 are slack variables, and hence the above problem can be recast to

$$\min x_1,
 x_1^2 + a \ge 0,
 x_1 - b > 0.$$
(55)

Benson, Shanno and Vanderbei (2004) have shown that even starting from the above neater form the interior-point method still faces the difficulty of jamming. Then, they proposed three possible solutions of the jamming problem.

For this problem the resulting ODEs by the FTIM are

$$\dot{x}_{1} = \frac{-v_{1}}{1+t} (1 - 2\lambda_{1}x_{1} - \lambda_{2}),
\dot{\lambda}_{1} = \frac{-v_{2}}{1+t} \left[\sqrt{\lambda_{1}^{2} + (x_{1}^{2} + a)^{2}} - \lambda_{1} - (x_{1}^{2} + a) \right],
\dot{\lambda}_{2} = \frac{-v_{2}}{1+t} \left[\sqrt{\lambda_{2}^{2} + (x_{1} - b)^{2}} - \lambda_{2} - (x_{1} - b) \right].$$
(56)

Here we fix a = -1 and b = 1, and the exact minimal solution is $x_1 = 1$.

We apply the FTIM on this problem by starting from the initial conditions of $x_1 = 1.5$, $\lambda_1 = \lambda_2 = 0.1$ and with the following parameters: h = 0.01, $v_1 = 0.2$, $v_2 = -6$ and $\varepsilon_1 = 10^{-5}$. Through about one second of computational time, the results are given by $x_1 = 1.00148$, $\lambda_1 = 0.0348839$ and $\lambda_2 = 0.02554765$. The accuracy is in the third order.

3.4 Example 4

In this case we examine the polygon of maximal area, among polygons with $n_{\nu}=2$ sides and diameter smaller than 1 [Graham (1975)]. If (r_i, θ_i) are the coordinates of the vertices of the polygon, then we must maximize the following optimization problem:

$$f = \frac{1}{2}r_{1}r_{2}\sin(\theta_{2} - \theta_{1}),$$

$$r_{1}^{2} + r_{2}^{2} - 2r_{1}r_{2}\cos(\theta_{2} - \theta_{1}) \leq 1,$$

$$0 \leq r_{1} \leq 1,$$

$$0 \leq r_{2} \leq 1,$$

$$\theta_{1} \leq \theta_{2},$$

$$\theta_{2} \leq \pi.$$
(57)

The governing ODEs in the FTIM are:

$$\dot{r}_{1} = \frac{-v_{1}}{1+t} \left[\frac{1}{2} r_{2} \sin(\theta_{2} - \theta_{1}) + 2\lambda_{1} r_{1} - 2\lambda_{1} r_{2} \cos(\theta_{2} - \theta_{1}) + \lambda_{2} - \lambda_{4} \right],
\dot{r}_{2} = \frac{-v_{1}}{1+t} \left[\frac{1}{2} r_{1} \sin(\theta_{2} - \theta_{1}) + 2\lambda_{1} r_{2} - 2\lambda_{1} r_{1} \cos(\theta_{2} - \theta_{1}) + \lambda_{3} - \lambda_{5} \right],
\dot{\theta}_{1} = \frac{-v_{1}}{1+t} \left[\frac{-1}{2} r_{1} r_{2} \cos(\theta_{2} - \theta_{1}) - 2r_{1} r_{2} \lambda_{1} \sin(\theta_{2} - \theta_{1}) + \lambda_{6} \right],
\dot{\theta}_{2} = \frac{-v_{1}}{1+t} \left[\frac{1}{2} r_{1} r_{2} \cos(\theta_{2} - \theta_{1}) + 2r_{1} r_{2} \lambda_{1} \sin(\theta_{2} - \theta_{1}) - \lambda_{6} + \lambda_{7} \right],
\dot{\lambda}_{1} = \frac{-v_{2}}{1+t} \min[\lambda_{1}, 1 - r_{1}^{2} - r_{2}^{2} + 2r_{1} r_{2} \cos(\theta_{2} - \theta_{1})],
\dot{\lambda}_{2} = \frac{-v_{2}}{1+t} \min[\lambda_{2}, 1 - r_{1}],
\dot{\lambda}_{3} = \frac{-v_{2}}{1+t} \min[\lambda_{3}, 1 - r_{2}],
\dot{\lambda}_{4} = \frac{-v_{2}}{1+t} \min[\lambda_{4}, r_{1}],
\dot{\lambda}_{5} = \frac{-v_{2}}{1+t} \min[\lambda_{5}, r_{2}],
\dot{\lambda}_{6} = \frac{-v_{2}}{1+t} \min[\lambda_{6}, \theta_{2} - \theta_{1}],
\dot{\lambda}_{7} = \frac{-v_{2}}{1+t} \min[\lambda_{7}, \pi - \theta_{2}].$$
(58)

We apply the FTIM to this problem by starting from the initial conditions of $r_1 = r_2 = \theta_1 = \theta_2 = 0.9$, $\lambda_1 = \dots = \lambda_7 = 0.1$ and with the following parameters: h = 0.01, $v_1 = -0.1$, $v_2 = -33$ and $\varepsilon_2 = 10^{-4}$. Through 126 steps the result of the maximal value of f is given by 0.4332801, which is very close to the exact value $\sqrt{3}/4 = 0.4330127$. The accuracy is in the fourth order.

3.5 Example 5

In this example we calculate an optimal mixing policy of two catalysts governed by a nonlinear model that describes the reactions:

$$x'_{1}(\tau) = u(\tau)[10x_{2}(\tau) - x_{1}(\tau)],$$

$$x'_{2}(\tau) = u(\tau)[x_{1}(\tau) - 10x_{2}(\tau)] - [1 - u(\tau)]x_{2}(\tau),$$
(59)

where x_1' and x_2' are the differentials of x_1 and x_2 with respect to τ . We use the notation τ to represent the real time and t for the fictitious time. Initial conditions

are given by $x_1(0) = 1$ and $x_2(0) = 0$. The control variable u represents the mixing ratio of the catalysts and must satisfy the following bounds:

$$0 < u(\tau) < 1. \tag{60}$$

The problem is to minimize

$$-1 + x_1(\tau_f) + x_2(\tau_f), \tag{61}$$

where $\tau_f = 1$. This problem is a typical bang-singular-bang problem. The singularity leads to nonunique values of the control in the singular region, and thus it is possible to obtain different values for the control.

We divide the time interval of $\tau \in [0,1]$ into n-1 subintervals, that is, $\Delta \tau = 1/(n-1)$. Denote the values of x_1 , x_2 and u at the discretized times by $x_1^i = x_1(\tau_i) = x_1((i-1)\Delta\tau)$, $x_2^i = x_2(\tau_i) = x_2((i-1)\Delta\tau)$ and $u^i = u(\tau_i) = u((i-1)\Delta\tau)$. Then by using a backward difference, from Eqs. (59) and (60) we can obtain

$$\frac{x_1^i - x_1^{i-1}}{\Delta \tau} - u^i (10x_2^i - x_1^i) = 0,$$

$$\frac{x_2^i - x_2^{i-1}}{\Delta \tau} - u^i (x_1^i - 10x_2^i) + (1 - u^i) x_2^i = 0,$$

$$u^i \ge 0,$$

$$1 - u^i \ge 0.$$
(62)

Therefore, we come to a minimization problem with equality and inequality constraints, of which the Lagrangian is given by

$$L = -1 + x_1^n + x_2^n + \mu_1^i \left[\frac{x_1^i - x_1^{i-1}}{\Delta \tau} - u^i (10x_2^i - x_1^i) \right]$$

$$+ \mu_2^i \left[\frac{x_2^i - x_2^{i-1}}{\Delta \tau} - u^i (x_1^i - 10x_2^i) + (1 - u^i)x_2^i \right] - \lambda_1^i u^i - \lambda_2^i (1 - u^i).$$
 (63)

The governing ODEs in the FTIM are

$$\dot{x}_{1}^{i} = \frac{-v_{1}}{1+t} \left[\frac{x_{1}^{i} - x_{1}^{i-1}}{\Delta \tau} - u^{i} (10x_{2}^{i} - x_{1}^{i}) \right],
\dot{x}_{2}^{i} = \frac{-v_{1}}{1+t} \left[\frac{x_{2}^{i} - x_{2}^{i-1}}{\Delta \tau} - u^{i} (x_{1}^{i} - 10x_{2}^{i}) + (1 - u^{i})x_{2}^{i} \right],
\dot{u}^{i} = \frac{v_{2}}{1+t} \left[\mu_{1}^{i} (10x_{2}^{i} - x_{1}^{i}) + \mu_{2}^{i} (x_{1}^{i} - 10x_{2}^{i}) + \mu_{2}^{i} x_{2}^{i} + \lambda_{1}^{i} - \lambda_{2}^{i} \right],
\dot{\mu}_{1}^{i} = \frac{-v_{1}}{1+t} \left(\frac{\mu_{1}^{i}}{\Delta \tau} + \mu_{1}^{i} u^{i} - \mu_{2}^{i} u^{i} \right),
\dot{\mu}_{2}^{i} = \frac{-v_{1}}{1+t} \left[-10\mu_{1}^{i} u^{i} + \frac{\mu_{2}^{i}}{\Delta \tau} + 10\mu_{2}^{i} u^{i} + \mu_{2}^{i} (1 - u^{i}) \right],
\dot{\lambda}_{1}^{i} = \frac{-v_{1}}{1+t} \min(u^{i}, \lambda_{1}^{i}),
\dot{\lambda}_{2}^{i} = \frac{-v_{1}}{1+t} \min(1 - u^{i}, \lambda_{2}^{i}).$$
(64)

The index *i* runs from 2 to *n*, and when i = n, the right-hand sides of $\dot{\mu}_1^i$ and $\dot{\mu}_2^i$ are supplemented with $-v_1/(1+t)$.

All initial conditions of the evolutional variables are given by 0.5. Under the following parameters: n = 101, h = 1, $v_1 = 0.04$ $v_2 = -0.3$ and $\varepsilon_2 = 10^{-6}$, the FTIM converges within 2949 steps, where the minimal value of f is -0.047588. In Fig. 2 we plot the time histories of x_1 , x_2 and u. It is interesting that the control u obtained by the FTIM is more smooth than that obtained by other methods. It means that the present control obtained by the FTIM is more easy to perform than that obtained by other methods.

3.6 Example 6

In this example we calculate the inverse boundary value problems of elliptic type PDEs by using the formulation of optimization. It is known that the inverse Cauchy problem is very hard to calculate [Liu (2008f, 2008g)].

We first consider an analytical solution of Laplace equation:

$$u(x,y) = e^x \cos y. ag{65}$$

The domain is given by $\Omega = \{(x,y) | 0 \le x \le 1, \ 0 \le y \le 1\}$. The exact boundary data can be obtained by inserting the exact u on the boundary:

$$u(x = 0, y) = \cos y, \ u_x(x = 0, y) = \cos y,$$

 $u(x, y = 0) = e^x, \ u(x, y = 1) = e^x \cos 1.$ (66)

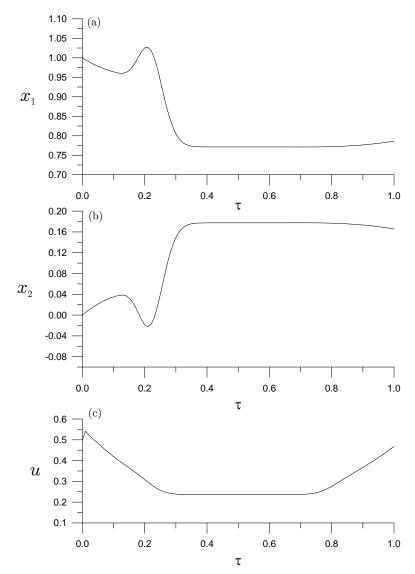


Figure 2: For Example 5 the time histories of x_1 , x_2 and u are plotted.

On the side of $x=0,\ 0\leq y\leq 1$ the data are overspecified; however, on the side of $x=1,\ 0\leq y\leq 1$ the data is not given, and we want to recover the data on this side. Let $\Delta x=\Delta y=1/(n-1)$, and denote the values of u at the discretized points by $u_{i,j}=u((i-1)\Delta x,(j-1)\Delta y)$. Because $u_{n,j},\ j=2,\ldots,n-1$ are unknowns, we can

find them by searching the minimization of

$$\min \frac{1}{2} \sum_{j=2}^{j=n-1} \left[u_{2,j} - u_{2,j}^e \right]^2, \tag{67}$$

where the exact data $u_{2,j}^e$ can be obtained by an approximation with $u_{2,j}^e = u_{1,j} + \Delta x \cos y_j = (1 + \Delta x) \cos y_j$. This minimization problem is subjected to the following constraint:

$$\frac{1}{(\Delta x)^2} [u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] + \frac{1}{(\Delta y)^2} [u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] = 0, \ i, j = 2, \dots, n-1.$$
(68)

By applying the FTIM we can derive the following ODEs:

$$\dot{u}_{i,j} = \frac{-v_1}{(1+t)(\Delta x)^2} [u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] - \frac{v_1}{(1+t)(\Delta y)^2} [u_{i,j+1} - 2u_{i,j} + u_{i,j-1}],$$

$$\dot{u}_{n,j} = \frac{-v_2}{1+t} [u_{2,j} - (1+\Delta x)\cos y_j].$$
(69)

We fix $\Delta x = \Delta y = 1/(n-1)$ with n = 21. In Fig. 3(a) we show the numerical and exact data on the boundary, where h = 0.001, $v_1 = -0.01$, $v_2 = 13$ and $\varepsilon_1 = 10^{-3}$ are used.

Next we consider a more complex case with:

$$\Delta u = 4u^3,\tag{70}$$

which has an exact solution:

$$u(x,y) = \frac{1}{x+y+1}. (71)$$

Therefore, the data used in the FTIM can be obtained.

By applying the FTIM we can derive the following ODEs:

$$\dot{u}_{i,j} = \frac{-v_1}{(1+t)(\Delta x)^2} [u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] - \frac{v_1}{(1+t)(\Delta y)^2} [u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] + \frac{4v_1}{1+t} u_{i,j}^3,
\dot{u}_{n,j} = \frac{-v_2}{1+t} \left[u_{2,j} - \frac{1}{1+y_j} + \frac{\Delta x}{(1+y_j)^2} \right].$$
(72)

In Fig. 3(b) we show the numerical and exact data on the boundary, where h = 0.001, $v_1 = -0.01$, $v_2 = 5$ and $\varepsilon_1 = 10^{-3}$ are used. From the above calculations it can be seen that the FTIM works very well to recover the unknown data, even for the highly-illposed inverse Cauchy problems.

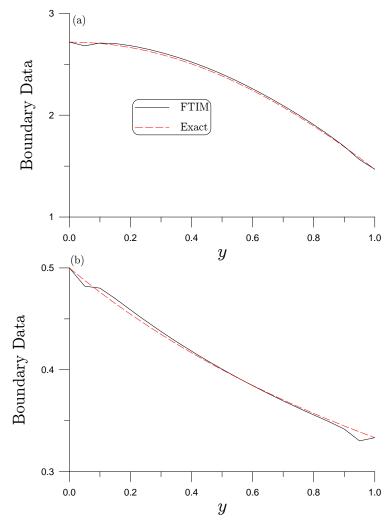


Figure 3: Comparing exact and numerical boundary data of Example 6.

3.7 Example 7

In this example we calculate a mixed complementarity problem due to an elastic-perfectly plastic model of material:

$$\sigma' = \varepsilon' - \lambda \sigma,$$

$$\sigma_0 - |\sigma| \ge 0,$$

$$\lambda \ge 0,$$

$$\lambda(\sigma_0 - |\sigma|) = 0,$$
(73)

where σ is a normalized stress, $\sigma_0=10^{-3}$ is a fixed normalized yield stress, and λ is a normalized dissipation rate. Similarly, τ is used to denote the real time.

We calculate this case by considering

$$\dot{\sigma} = \frac{-v_1}{1+t} [\sigma_i - \sigma_{i-1} - \Delta \tau \varepsilon'(\tau_i) + \Delta \tau \lambda_i \sigma_i],$$

$$\dot{\lambda} = \frac{-v_2}{1+t} [\sqrt{(\sigma_0 - |\sigma|)^2 + \lambda^2} - \lambda - \sigma_0 + |\sigma|].$$
(74)

We divide the total time span of the periodic strain input into 400 subintervals with $\Delta \tau = 20/400$, and the amplitude of strain rate is fixed to be 0.001. Under the following parameters of $v_1 = 30$, $v_2 = -1$ and $\varepsilon_1 = 10^{-6}$, we calculate the responses by using the FTIM. The hysteretic cycles and time history of dissipation rate are plotted in Fig. 4. When $\lambda = 0$ the material is in the elastic state, and when $\lambda > 0$ the material is in the plastic state.

4 Conclusions

The nonlinear optimization problems are transformed into the mixed-complementarity equations with the aid of Kuhn-Tucker conditions. Further the use of the NCP-functions leads to a set of nonlinear algebraic equations. The present paper very simply transforms the resulting nonlinear algebraic equations into an evolutionary system of ODEs by introducing a fictitious time, and by adding different coefficients v_i to enhance the stability of numerical integration of the resulting ODEs and to speed up the convergence of solutions. Because no inverse of a matrix is required, the present method is very time efficient. Several numerical examples of NOPs and MCPs were worked out. Some are compared with exact solutions revealing that high accuracy can be achieved by the FTIM. The present approach is simple and has a great advantage to easily extend to higher-dimensional NOPs with nonlinear equality and inequality constraints.

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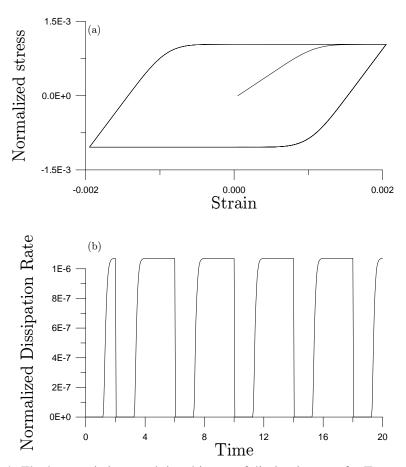


Figure 4: The hysteretic loop and time history of dissipation rate for Example 7 of plasticity.

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