Computational Methods for Differential Equations
http://cmde.tabrizu.ac.ir
Vol. 8, No. 4, 2020, pp. 661-672
DOI:10.22034/cmde.2020.33231.1537

Shortest Path Problem With Ordinary Differential Equations Constrained

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Abstract Many quick-link optimization models of transferring corrosive materials, need some constraints to change the output space such that all of the criteria are met, which forms a nonlinear problem with specific constraints. So we use an approach for finding global solutions of mixed-integer nonlinear optimization problems with ordinary differential equation constraints on the shortest path problem connective body composition because we need to save time. For the solution of constrained differential equations, we present a numerical method by coupling an implicit numerical method, and the results will be expressed by showing that the optimal path is selected.

Keywords. Implicit method, Shortest path, Constrained differential equations.

2010 Mathematics Subject Classification. 65L05, 34K06, 34K28.

1. Introduction

Some problems of optimization, involve both nonlinear dynamic systems and discrete decisions that affect the quality of the final plan. Decision problems are a kind of non-linear problem that is a combination of the difficulty of discrete variables and nonlinear functions. This problem is named mixed-integer nonlinear programming (MINLP) problems. This paper has connections to optimization with ordinary differential equations (ODE) or partial differential equation (PDE) constraints for a starting point into this area [3]. Optimisation problems and combine it with ODE are often used to describe systems dynamic behavior in many fields. In addition in some cases, the many phenomena of interest are nonlinear in nature and are described by systems of ODEs or by differential-algebraic equation (DAE) systems [4]. Differential constraints were introduced originally in the theory of partial and ordinary differential equations of the first order. In particular, Jacobi used differential constraints to find the total integral of the nonlinear equation and Konig applied them to the equation of the second order [2]. Some approach is to use the first discretize, then optimize approach. Discrete decisions are often handled by branch-and-bound. The α-BB

Received: 4 May 2019 ; Accepted: 20 May 2019.
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method for Nonlinear Programming (NLP) was introduced by Adjiman [5, 6] and Sager [8] applied the convexification method to handle discrete decisions over time and show how to efficiently compute feasible solutions. Papamichail and Adjiman consider parametric ODEs and construct approximations via the α-BB approach [9]. Using a relaxations method based on piecewise linearization is one of optimizing approach and general first discretize [7]. Bock, Kirches, and Meyer discuss problems in which the discrete decisions depend on the state variables and present a reformulation method for this kind of problem [1]. Global approaches are based on convex relaxations of the solution space. Singer and Barton consider convex relaxation methods for ODEs constrained and applied Branch-and-Bound to solve it [10, 11].

In this paper, we use some algorithms to solve nonlinear optimization problems as globally with ODE constraints. We consider problems of the following form [12]:

$$\begin{aligned} &\min\ C(x,\ y,\ z) \\ &s.t.\ G(x,\ y,\ z) \leq 0, \\ &\qquad \partial_k y(k) = f(k,\ x,\ y(k))\ ,\ k \in [0,\ K]\ (\mathcal{P}_{ode}) \\ &\qquad x \in X,\ y \in Y,\ z \in Z, \end{aligned} \tag{1.1}$$

where $X \subset \mathbb{R}^l$ and $Y \subset \mathbb{R}^n$ are polytopes and $Z \subset \mathbb{Z}^m$ is bounded. Furthermore, the objective function is $C : X \times Y \times Z \to \mathbb{R}$ and constraints are given by $G : X \times Y \times Z \to \mathbb{R}^s$. Thus, the variables $y(k)$ are functions that have to solve an ODEs specified by the function $f : \mathbb{R} \times \mathbb{R}^k \times \mathbb{R}^n \to \mathbb{R}^n$. Moreover, continuous variables x and integer variables z are present. If we consider 0 and K as the beginning and end of the interval, we can have two conditions on continuous variable y, so that y in objective function and differential constrained changes to $y^0,\ y^K$ $(C(x,\ y^0,\ y^K,\ z))$. So we have

$$\begin{aligned} &y^0 = y(0),\ y^K = y(K)\ , \\ &y^0 \in Y^0,\ y^K \in Y^K. \end{aligned}$$

Also, we assume that C, G, and f are continuously differentiable. So, the differential equations are made by n one-dimensional ODEs $\partial_k y_i(k) = f_i(k,\ x,\ y_i(k))$ for $i = 1, \ldots, n$, one for each of the n pipelines in the corresponding network. We will use a solution method to globally solve, and we will implement the example of connective body composition with the shortest path problem to illustrate the approach.

The remainder of this paper is organized as follows. In Section 2, the solution method is defined for the problem. Section 3 provides a brief introduction to interval analysis and Taylor models, as well as a constraint propagation procedure on Taylor models. Section 4 reviews the new validated method for parametric ODEs, which makes use of Taylor models. Section 5 then outlines the algorithmic procedure for solving the global optimization problem. Finally, in Section 6, we present the results of some numerical experiments that demonstrate the effectiveness of the proposed approach for parameter estimation of dynamic systems.

2. Solution Method for ODE Constrained Problem

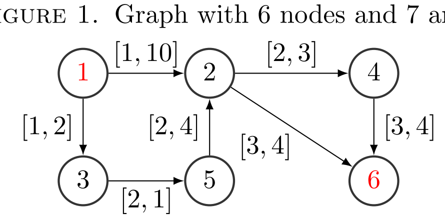
The shortest path problem (SPP) involves the constrained shortest path problem in a specified graph where the arc resources are determined, and the objective is finding the shortest path from an initial node to an end node. In most routing and crew scheduling applications where they generate with some subproblem corresponds to the shortest path problem with resource constraints (SPPRC). We know that in the deterministic SPP all the parameters such as distance, time or cost are known. So consider the SPP as follows

$$\begin{aligned} &\min\ c^T x \\ &s.t: Mx = b, \\ &\qquad x \in \{0,1\}^n. \end{aligned}$$

Note that this model only has one source, on the other hand, $x \in \{0,1\}^n$ means that if there is a path from one node to another node x will be 1, otherwise 0. We consider $M_{m\times n}$ as a nod-arcs incidence matrix, where m, n are the number of nodes and arcs, respectively.

In the shortest path problems, in addition to the fact that the problem may have a source, other indicators can be considered in the problem. To illustrate what we will say later, we give an example in numerical form.

Figure 1. Graph with 6 nodes and 7 arcs.



This example shows a 6-point graph in which each edge consists of two indeces: the first one is cost and the second one is time. We try to minimize the cost of transfer from the source node to the destination. For this example, there is a differential equation in time, and in addition, the model must be satisfied in condition $t \leq 12$. Perhaps this question arises against, why the time is not considered as a objective function? Maybe your path has a shorter time, but the cost of transporting goods is not reasonable and expected. Therefore, we select a path that will be optimized for both of the indicators. We present a table for Figure 1, includes paths, costs, and times information.

	Paths	Costs	Times
1	$1 \to 2 \to 6$	4	14
2	$1 \to 2 \to 4 \to 6$	5	10
3	$1 \to 3 \to 5 \to 2 \to 6$	8	12
4	$1 \to 3 \to 5 \to 2 \to 4 \to 6$	9	13

TABLE 1. Table of paths, costs, and times information for every path. Optimal time is $t \leq 12$.

Path number 2 is optimal. Note that path 1 has a lower cost, but the passage time is not optimal, and in path 3, while the time is optimal, the cost is too high. Therefore, path 2 has been selected with optimal cost and time.

3. ODE Model

In this section, we will present the SPP model with a ODE constraint as follows

$$\begin{aligned}
&\min\, c^T x \\
&s.t: Mx = b, \\
&\qquad \frac{dy}{dt} = f(t, y(t)), \\
&\qquad g(x) \leq 0, \\
&\qquad y(0) = y^0, \\
&\qquad x \in \{0,1\}^n, \\
&\qquad y(0) \in Y^0,
\end{aligned} \tag{3.1}$$

where $Y^0 \in \mathbb{R}^n$.

In the numerical example section, the time constraint will also be added. According to reference [12], the authors are trying to approximate differential constraints by using a convex function below the ODE constraint curve and a concave function above the ODE constraint, but in this article, we have done differently. Since for our example with more attention to local truncation error, the trapezoidal numerical method is an upper bound on the differential equation and the Euler implicit methods, explicit Euler, and the midpoint method are lower bound on the differential equation, therefore, instead of convex and concave functions, a favorable upper bound and lower bound are used.

Before examining numerical methods, there are some discussions about the properties of the initial value-problem of

$$\begin{aligned}
&\frac{dy}{dt} = f(t, y(t)), \\
&y(0) = y^0,
\end{aligned} \tag{3.2}$$

including the concepts of existence and the unique solution.

Theorem 3.1. [13] *Suppose D is a open-connected set from $\mathbb{R}^2$, $f(t, y(t))$ be a continuous function from y to t for all $(t, y) \in D$. Assume (t_0, y_0) is a interior point of D. if $f(t, y)$ satisfies on Lipschitz condition, such as*

$$| f(t, y_1) - f(t, y_2) | \leq K | y_1 - y_2 |, \ \forall (t, y_1), (t, y_2) \in D, \tag{3.3}$$

then there is a uniquely function $Y(t)$ defined on the interval $[t_0 - \alpha, t_0 + \alpha]$ where $\alpha > 0$, which satisfies to the following problem

$$\begin{aligned} &Y^{'}(t) = f(t, Y(t)), \ t_0 - \alpha \leq t \leq t_0 + \alpha, \\ &Y(t_0) = Y_0. \end{aligned}$$

In the theorem (3.1), the Lipschitz condition was expressed for f. If $\dfrac{df(t, y)}{dt}$ is a continuous function of (t, y) in $\overline{D}$ (closure of D) with D convex, obviously inequality (3.3) is derived. In this case with a finite condition, we can use

$$K = \max_{(t,y)\in\overline{D}} \ | \frac{df(t, y)}{dt} | \, .$$

Otherwise, it is easy to use a smaller set of D, including $(t-0, Y_0)$, which is bounded. The value of α in the theorem (3.1) depends on the initial value-problem of (3.2). For some equations such as the linear equation, the solution exists for every t, and α can be considered infinite. For many nonlinear equations, the solution is only available in a bounded interval.

Assume $F : T \times Y^0 \to \mathbb{R}^n$ and $(t, y^0) \to y(t)$. Then we can replace ODE constraint with

$$y^t - F(t, y^0) = 0.$$

Then, the model (3.1) will be change as follows

$$\begin{aligned} &\min \ c^T x \\ &s.t : Mx = b, \\ &\quad\ \ y^t - F(x, y^0) = 0, \\ &\quad\ \ g(x) \leq 0, \\ &\quad\ \ x \in \{0, 1\}^n, \\ &\quad\ \ y(0) \in Y^0. \end{aligned} \tag{3.4}$$

Assumption 3.2. [12] *There exist functions $F^l : T \times Y^0 \to \mathbb{R}^n$ and $F^u : T \times Y^0 \to \mathbb{R}^n$, which fulfill the inequality*

$$F^l(t, \ y^0) \leq F(t, \ y^0) \leq F^u(t, \ y^0),$$

for all $t \in T$ and $y^0 \in Y^0$. In addition, we assume that on the polytopes T, Y^0 the functions F_i^l and F_i^u converge uniformly to F_i for $N_i \to \infty, i = 1, \ldots, n$.

FIGURE 2. Existence and stability of the method.

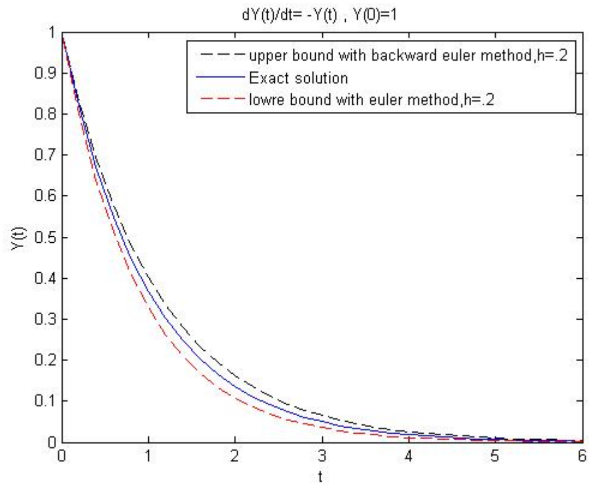


Figure 1 shows that for every ODE constraint, e.g. $y^{'}(t) = -y(t)$, we can find numerical methods that satisfied in $F^l \leq y(t) \leq F^u$. For this example, we present lower bound with Euler numerical method and upper bound with the backward Euler numerical method.

How we can know there exist functions F^l and F^u, which satisfy Assumption (3.2)? We suppose an one-dimensional ODE

$$y(0) = y^0,\ \partial_t y(t) = f(t,\ y(T))\ ,\ t \in [0,\ T],$$

with usage implicit one-step methods (Euler) with the length of step we can write

$$y_0 = y^0,\ y_{i+1} = y_i + h_i f_h(t_i,\ h_i,\ y_i,\ y_{i+1})\ ,\ \forall i = 0,\ \ldots,\ N-1, \tag{3.5}$$

subject to t_i is increased, then we have

$$0 = t_0 < t_1 < \cdots < T_N = T.$$

Define steps with $h_i := t_{i+1} - t_i,\ \forall i = 0, \ldots, N-1$. The case that is important is the definition of F^l and F^u using equation (3.5)

$$F^l : y^0 \mapsto y_N,$$

and or

$$F^u : y^0 \mapsto y_N.$$

The goal is to get the lower and upper bounds at $y(L)$ and close together so that the gap between the two borders is minimized.

To analyze the error, assume that the initial value problem has a unique solution of $Y(t)$ on $t_0 \leq t \leq b$ and also, this solution has a boundary second derivative $Y^{''}(t)$ on this interval. We start the discussion by applying Taylor's theorem for approximation (3.2)

$$Y(t_{n+1}) = Y(t_n) + hY^{'}(t_n) + \frac{1}{2}h^2 Y^{''}(\xi_n),$$

where $t_n \leq \xi_n \leq t_{n+1}$. Given that $Y(t)$ is the solution to the differential equation, we can write

$$Y^{'}(t) = f(t, Y(t)).$$

Using Taylor approximation

$$Y(t_{n+1}) = Y(t_n) + hf(t_n, Y(t_n)) + \frac{1}{2}h^2 Y^{''}(\xi_n), \tag{3.6}$$

where the sentence

$$T_{n+1} = \frac{1}{2}h^2 Y^{''}(\xi_n), \tag{3.7}$$

is named truncation error of Euler method. To analyze error in the Euler's method, we can write

$$Y(t_{n+1}) - y_{n+1} = Y(t_n) - y_n + h[f(t_n, Y_n) - f(t_n, y_n)] + \frac{1}{2}h^2 Y^{''}(\xi_n), \tag{3.8}$$

where $y_{n+1} = y_n + hf(t_n, y_n)$. Therefore, we use the local truncation error

$$Y(t_n) - y_n + h[f(t_n, Y_n) - f(t_n, y_n)] \geq 0. \tag{3.9}$$

Lemma 3.3. [12] *Consider a method of the form* (3.5) *for a scalar ODE,* $y(t) \in \mathbb{R}$, *and let the local truncation error of the method be nonnegative, the inequality*

$$y(s+h) - y(s) - hf_h(s,\ h,\ y(s),\ y(s+h)) \geq 0,$$

holds for all $s \in [0,\ S]$ *and* $h \geq 0$ *with* $s + h \leq S$*. Suppose the derivatives satisfy*

$$b \leq \partial_y f_h(s,\ h,\ y,\ \mathrm{y}),$$

and

$$\partial_{\overline{y}} f_h(s,\ h,\ y,\ \mathrm{y}) \leq B,$$

for constants $b, B \in \mathrm{R}$*. Then if*

$$0 < h_i \leq h_{\max} = \left\{ \begin{array}{cl} \infty & \textit{if}\ \ b \geq 0 \textit{ and } B \leq 0 \\ \frac{1}{\max\{-b, B\}} & \textit{if otherwise} \end{array} \right. ,$$

for all $i = 1, \ldots, N$*, the one-step method produces a lower bound on the solution* $y(t)$ *, i.e.,*

$$y_i \leq y(t_i), i = 1, \ldots, N,$$

if on the other hand the local truncation error of the method is nonpositive, i.e., the inequality

$$y(t+h) - y(t) - hf_h(t, h, y(t), y(t+h)) \leq 0,$$

holds for all $t \in [0, T]$ *and* $h \geq 0$ *with* $s + h \leq S$*, then we obtain under the same assumptions*

$$y_i \geq y(t_i), i = 1, \ldots, N.$$

Lemma 3.4. [12] *If we consider an explicit one-step method, i.e., $f_h(t, h, y, \mathrm{y})$ is independent of* y, *that is $y_{i+1} = y_i - h_i f_h(t_i, h_i, y_i)$, then the previous lemma yields that we can choose*

$$h_{\max} = \begin{cases} \infty & \mathit{if}\, b \geq 0 \\ -\frac{1}{b} & \mathit{else} \end{cases}.$$

Remark 3.5. [12] If we consider an "end value problem" instead of an initial value problem, ($\partial_t y(t) = f(t,\ y(t))$ holds for $t \in [0,\ T]$ and $y(T) = y^T$) then, Lemma 7 still holds true with the modification, where the bounds are now reversed, i.e. positive truncation error now yields upper bounds and negative truncation error now yields lower bounds.

Consider the following model given that the ODE constraint is a function of time

$$\min c^T x \tag{3.10}$$
$$s.t : Mx = b, \tag{3.11}$$
$$x \in \{0, 1\}^n, \tag{3.12}$$
$$\frac{dT}{dt} = f(t, T(t)), \tag{3.13}$$
$$T(0) = T^0, \tag{3.14}$$
$$T = \overrightarrow{Time} \bullet x, \tag{3.15}$$
$$T(t) \geq z. \tag{3.16}$$

For the model (3.10), steps of the solution are as follows

The SPP to use in this whole article is based on minimizing the cost. Now, we want to present a model that aims to minimize time. The related cost condition is considered as a constraint.

$$\min T \tag{3.17}$$
$$s.t : c^T x \leq C,\ Mx = b,\ x \in \{0, 1\}^n, \qquad (SPPconstraint) \tag{3.18}$$
$$\frac{dT}{dt} = f(t, y(t)), \tag{3.19}$$
$$t = \overrightarrow{time} \bullet x, \tag{3.20}$$
$$T(0) = T^0, \tag{3.21}$$
$$T(t) \geq z. \text{ (z is temperature parameter)} \tag{3.22}$$

Algorithm 1: Calculate shortest path problem with ODE constraints

INPUT: $c, M, b, z, \overrightarrow{Time}$
OUTPUT: $T(t), c^T x, x$
STEP 1:
first solve the shortest path problem without considering the ODE constraints(15-18)(I).
$\min\ c^T x$
$s.t:\ Mx = b$
$cx \geq 0$
$x \in \{0, 1\}$
and get x^* as a optimal solution
STEP 2:
paste the obtained x into the following conditions (II).
$F^l \leq T^t \leq F^u$
$T(0) = T^0$
$T = \overrightarrow{Time} \bullet x$
$T(t) \geq z$
if x satisfied in conditions (II)
go STEP 3
else
replace $cx \geq cx^*$ with $cx \geq 0$ and solve model (I)
go STEP 2
END

Algorithm 2: Calculate shortest path problem with ODE constraints

INPUT: $c, M, b, z, \overrightarrow{time}$
OUTPUT: $T(t), x$
first solve ODE constraint with a numerical methods where points are equidistant.
obtain F^l, F^u functions
$F^l \leq T(t) \leq Fu$
if F^l be convex
solve model (3.17) with constraint $F^l \leq T(t)$
else if
F^u be concave
solve model (3.17) with constraint $T(t) \leq F^u$
else
$T(t)$ yields an approximate solution of the equation that don't necessarily calculate the upper and lower bound then select a constraint between $F^l \leq T(t)$ and $T(t) \leq F^u$ and solve model (3.10).

4. Numerical Example

One of the issues that we are facing today is the transport of corrosive materials, e.g. transport of transplantation's organ, from one point to the next. We know for that matter the most important thing is the rapid arrival of the materials to the destination to prevent corruptions. So time is one of the factors that arise in this issue. In addition to this, the transfer will lead to a cost in any way that goes through. Then, we need the cost of transferring as low as possible. The goal is to find the shortest path. An example is presented in this section, which consists of $|V| = 12$ (nodes) and $|E| = 17$ (edges). Suppose that the material can be used up to a certain temperature. First, we heat the material up to 120 °C (°C is Degree Celsius). If the environment temperature is 25° C, the temperature changes with respect to time are as follows:

$$\frac{dT}{dt} = k(T - 25),$$

where $K = -0.346573$ for this type of material. The network is supposed to be an oriented network. For directions, $a_i \to a_j \quad s.t : i < j$. The input generated as follows

Figure 3. Graph with 12 nodes and 17 arcs.

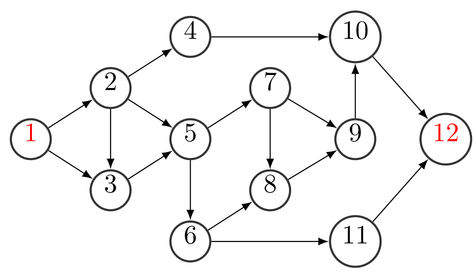


Table 2. Forward Euler for lower bound and backward Euler for upper bound; model (3.10).

	z	Optimal values	$F^u - F^l$	CPU (s)
h=0.2	27	$c^T x{=}18,\ t{=}10$	0.7	0.9710
	25	$c^T x{=}15,\ t{=}47$	9.4804e-06	0.4174
h=0.02	27	$c^T x{=}18,\ t{=}10$	0.0713	0.9117
	25	$c^T x{=}15,\ t{=}47$	9.0761e-07	0.4376
h=0.005	27	$c^T x{=}18,\ t{=}10$	0.0178	1.6073
	25	$c^T x{=}15,\ t{=}47$	2.2630e-07	0.4805
Optimal path: $z = 25$; $1 \to 2 \to 4 \to 10 \to 12$.				
Optimal path: $z = 27$; $1 \to 3 \to 5 \to 7 \to 9 \to 10 \to 12$.				

Table 3. Trapezoidal numerical method for lower bound and backward Euler for upper bound; model (3.10).

	z	Optimal values	$F^u - F^l$	CPU (s)
h=0.2	27	$c^T x{=}18,\ t{=}10$	0.3654	0.7908
	25	$c^T x{=}15,\ t{=}47$	5.9163e-06	0.3438
h=0.02	27	$c^T x{=}18,\ t{=}10$	0.0357	0.8502
	25	$c^T x{=}15,\ t{=}47$	4.6576e-07	0.3679
h=0.005	27	$c^T x{=}18,\ t{=}10$	0.0089	0.8636
	25	$c^T x{=}15,\ t{=}47$	21.1391e-07	0.4055

Table 4. Forward Euler for lower bound and backward Euler for upper bond; model (3.17).

	Lower bound	Upper bound	$F^u - F^l$	CPU (s)
$h{=}0.2,\ c^T x{=}18$	2.4883	3.0517	0.2299	0.0911
$h{=}0.02\ c^T x{=}18$	2.6915	2.7459	0.0266	0.1345
$h{=}0.005\ c^T x{=}18$	2.7115	2.7251	0.0067	0.0932

All the experiments were carried out on a PC with windows system and Intel(R) Core(TM) i7-7700K CPU@ 4.20 GH_z and 8Gb of RAM. Also, example solved in Matlab by mosek solver.

Conclusion

A numerical method for the differential equations coupled with a global optimization problem was investigated. Table 2 and Table 3 has presented a different numerical method for the lower and upper bound. According to the results, a trapezoidal numerical method provides a better result and the difference between the upper and lower bounds is at the lower level. The results show that we have been able to find a path, that in addition to the shortest path, time and cost are at the best predicted.

Acknowledgments

The authors would like to thank Dr. Rashed Khanjani Shiraz (University of Tabriz) for fruitful discussions and helpful comments and thanks for all those who have trusted us.

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