NUMERICAL CALIBRATION OF SCALAR CONSERVATION LAW MODELS USING REAL CODED GENETIC ALGORITHM

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Abstract. This article deals with the flux identification problem in scalar conservation laws. The problem is formulated as an optimization problem, where the objective function compares the solution of the direct problem with the observed profiles at a fixed time. A finite volume scheme solves the direct problem and a continuous genetic algorithm solves the inverse problem. The numerical method is tested with synthetic experimental data. The simulation parameters can be recovered approximately. The error depends on the parameters of the numerical scheme.

1. Introduction

The problem of flux identification in conservation laws is highly relevant in many fields of science and engineering, see for instance [1, 2, 3, 4, 5, 6] for sedimentation model, [7, 8] for chromatography model, [9] for centrifugation model, [10, 11] for flow through porous media model, [12] for highway traffic flow model and [13, 14] for analytical results. In a broad sense, the common starting point in all of these models, is that they are deducted in the context of continuum mechanics approach together with some appropriate assumptions and simplifications of the particular physical system. The result of this processes is a governing equations (often a system of conservation laws) closed under state laws or constitutive equations (algebraic relations for the flux function) and initial-boundary conditions. Typically, the initial and boundary conditions are estimated by measurements. Whereas that, the constitutive functions are determined qualitatively by phenomenological assumptions and quantitatively by the available information on experimental data. Often, the constitutive equations depend of unknown parameters which are not accessible by experimental determination or needs a very expensive (or complicated) laboratory tests. Therefore, in the framework of flux calibration, the following inverse problem is considered: given an observation of the model unknowns at a fixed time find the flux function such that the entropy solution for an initial-boundary value problem of a system of conservation laws is as close as possible to the observed data. Usually, the solution of this problem can be performed by optimization techniques, where the considered cost function quantifies the difference between the simulated and observed solutions.

In general, the solution of nonlinear conservation laws depends nonlinearly on the parameters and also develops discontinuities in finite time, independent of the regularity of the coefficients and the initial and boundary conditions [15]. This kind of behavior of the direct problem implies that, in most of the cases, the cost function turns out to be a non-convex and a nondifferentiable function (see for instance Figures 2 and 5). Thus, the inverse problem analysis can be developed following the nonconvex and nondifferentiable optimization theory. At this point, the application of numerical optimization tools fall into the two big kind of optimization methods: deterministic

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and stochastic, depending on the knowledge of the parameters. First, when there is some history about the parameter values a local minimum of the cost function can be find by deterministic methods. This kind of strategy has been considered by several authors, see [3, 4, 7, 16]. There, the central and common points are: they assume local convexity of the cost function close to a historical parameter value and introduce a formal calculus for the discrete gradient. Second, when there is not a history of the parameters to be estimated or, in the worst of the cases, there is not an intuitive estimation of the inverse problem solution, the use of stochastic optimization methods is suggested [17, 18, 19, 20, 21, 22, 23, 24].

Recently, an exhaustive and complete review of stochastic optimization methods applied to the inverse scattering problem was done by Rocca and coauthors in [22]. They reported a unified view of the evolutionary algorithms constructed under competitive or cooperative paradigms. For example, genetic algorithms are belongs to the former class, and swarm and ant colony algorithms are belongs the seconde ones. In particular, Rocca and collaborators make a clear description of the main features, disadvantages and the several important historical milestones of the nature-inspired evolutionary algorithms. For instance, in the case of genetic algorithms the properties are: (a) They imitate the principles of biological evolution for the construction of an iterative algorithm, (b) They are belong to the class of global methods which have the main advantage to depend neither explicitly nor implicitly on gradients, (c) They require only the evaluation of the cost function and promise a robust optimization. Hence, genetic algorithms usually work well in situations when gradient methods or gradient-like methods are found to fail in the sense of local convergence or nondifferentiability of the objective function. Furthermore, they conclude that, although the existing evolutionary algorithms are reliable and efficient in the tested inversion problems is of paramount importance for the theoretical development the implementation of this methodologies in new situations. Therefore, following this suggestion, we study a genetic algorithm for the flux identification problem in nonlinear scalar conservation laws.

On the other hand, concerning to the specific application of genetic algorithms to inverse problems in conservation laws, there are a few results available on the literature (see [24, 25, 26, 27]). First, in [24] the authors present a review of the algorithms used for the inverse problem arising in porous media and well-known as the history matching problem. In [25], the authors recover the coefficients of a linear one-dimensional model for the flow through porous media and include an extensive discussion about the benefits of genetic algorithms in contrast to more traditional gradient-based techniques. Now, in [26] a genetic algorithm is applied to identify the flux of a system of conservation laws of Saint-Venant type and modelling the flow on a river network. Meanwhile, in [27] the relative permeabilities defining the fractional in the BuckleyLeverett equation are reconstructed. We note that [25, 26, 27] is used a binary coded genetic algorithms. In addition, we mention also, that a new strategies of evolutionary was used in [28] to identify the flux in the Chromatography system. Thus, this paper is the first application of a real coded genetic algorithm.

In order to investigate the feasibility and applicability of the continuous genetic algorithm, we show three numerical examples. Although, the results of this paper are preliminary, and as far to solve the general inverse problem, we have some observed some good properties which delimits and makes the guidance of further development in more complex situations. First, we note that the agreement of observed and the identified parameters by the algorithm has high quality. Furthermore, it was observed that the extremum of the numerical cost function depends on the order of the finite volume method used for the discretization of the direct problem. In this sense, we believe that the application of the algorithm with a high resolution numerical method for the direct problem solution contributes naturally to several improvements to the numerical flux identification in conservation laws. Thus, the numerical examples given in this article clearly suggest that the use of genetic algorithms is a powerful numerical tool for parameter identification in conservation laws. However, before of the application of more complex scenarios of theoretical or engineering interest, some items must be improved. For instance, it will be useful the development of the hybrid algorithms with combination of the continuous genetic algorithm with other evolutionary strategies and even with the deterministic algorithms. Moreover, in the case of explicit finite

volume schemes for the forward simulations is highly needed the parallelization of the genetic algorithm.

The paper is organized as follows. In Section 2, we introduce the continuous direct and inverse problems and their discretization. In Section 3, we present the continuous genetic algorithm. Finally, in Section 4, we document the numerical results.

2. Continuous direct-inverse problem and Discretization

In this section we precise the definitions of the direct and inverse problems, the parameter identification problem, the discretization of the direct problem and the definition of the discrete cost function.

2.1. Direct an inverse problem.

The direct problem is given by the following initial boundary value problem

$$\begin{aligned} u_t + (f(u))_x &= 0, \ \ (x,t) \in Q_T := I \times \mathscr{T}, && (2.1)\\ u(x,0) &= u_0(x), \ \ x \in I := (0,1), && (2.2)\\ u(\ell,t) &= g_\ell(t), \ \ \ell \in \{0,1\}, \ \ t \in \mathscr{T} := [0,T], && (2.3) \end{aligned}$$

where t denotes time, x the spatial variable, u the state variable, f the flux function, u_0 is the initial condition, and $g_\ell,\ \ell \in \{0,1\}$ are the boundary conditions. Typically, we assume that u_0, f, g_0 and g_1 are given functions and we want to find $u(\cdot,T)$ in a finite time $T > 0$. However, often f in unknown and should be determined by the solution of an inverse problem. This inverse problem is the well-known calibration problem, where a set of experimental is considered in order to have an overspecified problem. For instance, assuming that $\hat{u}(x)$ is a given experimental solution profile in a fixed time $t = T$. Thus, the inverse problem of flux identification can be formulated as the following optimization problem

$$\begin{cases} \text{minimize} & J(u) := \dfrac{1}{2}\displaystyle\int_{\mathscr{I}} \left|(u-\hat{u})(x)\right|^2 dx, \\ \text{subject to} & E(u,p;f) = 0, \quad f \in U_{\text{ad}}, \end{cases} \tag{2.4}$$

where the the constraint $E(u,p;f)$ is the weak integral formulation of the direct problem (2.1)-(2.3)

$$\begin{aligned} E(u,p;f) = &- \int\int_{Q_T} \Big\{ up_t + f(u)p_x \Big\}\, dx\, dt \\ &+ \int_{\mathscr{T}} \Big\{ f(g_1(t))p(1,t) - f(g_0(t))p(0,t) \Big\}\, dt - \int_{\mathscr{I}} u_0(x)p(x,0)\, dx, \end{aligned}$$

for all $p \in C_0^1(Q_T)$ and U_{ad} is the flux admissible set defined

$$\mathscr{U}_{ad} = \Big\{ f : \mathbb{R} \to \mathbb{R} \ \Big|\ f \in C^2(\mathbb{R}),\ f(0) = f'(0) = 0,\ f''(u) > 0 \quad \forall\, u \in I_{\max} \Big\},$$

on the maximum interval $I_{\max} = \Big[\min(A), \max(A)\Big]$ with $A = \Big\{ \|u_0\|_{L^\infty(I)}, \|g_1\|_{L^\infty(\mathscr{T})}, \|g_2\|_{L^\infty(\mathscr{T})} \Big\}$. Here, note that the optimization problem (2.4) allows to determine the flux function belongs to $\mathscr{U}_{ad}$ that matches best to the observation data. The definition of $\mathscr{U}_{ad}$ is fundamental for the genetic algorithm, since it determines the trial region of the parameter space where the initial population is sampled. Furthermore, note that the set $\mathscr{U}_{ad}$ denotes all convex flux functions and should be redefined in the case of more general flux functions, for instance in the case of sedimentation where f is a nonconvex flux function with a single or with two inflection points.

2.2. Parameter identification problem.

For the parameter identification problem we assume that the flux function depends on a finite number of parameters, denoted by $\mathbf{e} = (e_1, \ldots, e_d) \in \mathbb{R}^d$, i.e. $f(\cdot) = f(\cdot;\mathbf{e})$. Typically, the analytical parametric dependence of the flux function f on the parameter set $\mathbf{e}$ comes from a constitutive relation between the velocity and the density. For instance, in the case of traffic flow modeling, it is assumed that the flux function is defined by $f(u) = uv(u)$, where v is the velocity. For example, in the Lighthill-Whitham model for traffic flow the velocity is given by $v(u) = v_*\,(1 - u/\rho^*)$, such that v_* and ρ^* are the parameters for the calibration by (2.5), see [29, 30] and Example 4.2 below. Thus, the general formulation of the

optimization problem (2.4) is reduced to an optimization problem with respect to d-parameters as follows

$$\begin{cases} \text{minimize} & \mathscr{J}(\mathbf{e}) := J\Big(u(\mathbf{e})\Big), \\ \text{subject to} & E\Big(u(\mathbf{e}), p; f(u(\mathbf{e}); \mathbf{e})\Big) = 0, \\ & \mathbf{e} \in D := \{\mathbf{x} \in \mathbb{R}^d : f(u; \mathbf{x}) \in \mathscr{U}_{\text{ad}} \text{ for all } u \in I_{\max}\}. \end{cases} \tag{2.5}$$

The set $D \subset \mathbb{R}^d$ represents the largest set such that the flux is belongs to $\mathscr{U}_{\text{ad}}$ and is the natural set for the global search of the optimization algorithm.

2.3. **Numerical solution of direct problem.** Let us first recall the standard notation of finite volume methods for conservation laws (see [29, 31, 32] for more details). We subdivide the spatial domain $\mathscr{I}$ into M subintervals K_i of length $\Delta x = 1/M$ centered at $x_j = j\Delta x$, for $j = 0, \ldots, M$, and defined by $K_j := (x_{j-1/2}, x_{j+1/2})$. Here $x_{j+1/2} = (x_j + x_{j+1})/2$ for $j = 0, \ldots, M-1$, $x_{-1/2} = x_0 - \Delta x/2$ and $x_{M+1/2} = x_M + \Delta x/2$. The sets K_j are called the cells or control volumes and its boundaries are called interfaces. Similarly, the temporal domain $\mathscr{T}$ is partitioned into N subintervals of length $\Delta t = T/N$ and defined by $R_n = [t_n, t_{n+1})$, where $t_n = n\Delta t$, for $n = 0, \ldots, N$. For notational simplicity we set $Q_j^n := K_j \times R_n$ and the numerical solution of (2.1)-(2.3) over Q_j^n is denoted by u_j^n. With this notation at hand, we discretize the equations (2.1)–(2.3). Indeed, we start with the discretization of the initial condition (2.2)

$$u_j^0 = \frac{1}{\Delta x} \int_{K_j} u_0(x)\, dx, \quad j = 0, \ldots, M. \tag{2.6}$$

Then, following the ideas of finite volume technique, we integrate over Q_j^n the equations (2.1)-(2.3) and deduce the following numerical scheme

$$u_j^{n+1} \;=\; u_j^n - \lambda\Big\{f_{j+1/2}^n - f_{j-1/2}^n\Big\}, \quad \lambda = \frac{\Delta t}{\Delta x}, \quad f_{j+1/2}^n \approx \frac{1}{\Delta t} \int_{R_n} f(u(x_{j+1/2}, t))dt, \tag{2.7}$$

for all $n = 0, \ldots, N$ and $j = 0, \ldots, M$, where $f_{j+1/2}^n$, in the case of $2p+1$ points scheme, may be written as follows: $f_{j+1/2}^n = g(u_{j-p+1}^n, \ldots, u_{j+p}^n)$ with $g \in \text{Lip}(\mathbb{R}^{2p}, \mathbb{R})$ and $g(u, \ldots, u) = f(u)$. The function g is called the numerical flux function and the last property of g is known as the consistence for the finite volume scheme (2.7). A particular and interesting case are the well-known monotone flux schemes, where $g : \mathbb{R}^2 \to \mathbb{R}$ satisfies the following assumptions [31]:

- (G1) *Lipschitz-regularity.* g is locally Lipschitz with respect to each of its variables on $[u_m, u_M]^2$,
- (G2) *Consistence.* $g(u, u) = f(u)$, for all $u \in [u_m, u_M]$,
- (G3) *Monotonicity.* g is non-decreasing with respect to its first variable and non-increasing with respect to its second variable on $[u_m, u_M]^2$.

The explicit monotone flux schemes have played a very important role in the development of numerical analysis for conservation laws due to their good properties: consistence in the finite volume sense, L^∞-stability, BV-stability and convergence of the numerical solution to the entropy solution under a CFL condition, see [31, 29] for further details. To be precise, in the numerical simulations given in this paper, we consider the numerical flux of Godunov, which is defined for $f \in \mathscr{U}_{\text{ad}}$ by the following explicit relation

$$g^{\text{God}}(u, v) := \begin{cases} f(u), & u \geq 0 \quad \text{and} \quad v \geq 0, \\ f(v), & u \leq 0 \quad \text{and} \quad v \leq 0, \\ \min\Big\{f(u), f(v)\Big\}, & u \leq 0 \leq v, \\ \max\Big\{f(u), f(v)\Big\}, & v \leq 0 \leq u. \end{cases} \tag{2.8}$$

and naturally (2.7) is written as follows

$$u_0^{n+1} \;=\; u_0^n - \lambda\Big\{g^{\text{God}}(u_0^n, u_1^n) - f(u_0^n)\Big\}, \tag{2.9}$$

$$u_j^{n+1} \;=\; u_j^n - \lambda\Big\{g^{\text{God}}(u_j^n, u_{j+1}^n) - g^{\text{God}}(u_{j-1}^n, u_j^n)\Big\}, \tag{2.10}$$

$$u_M^{n+1} \quad = \quad u_M^n - \lambda\Big\{f(u_M^n) - g^{\mathrm{God}}(u_{M-1}^n, u_M^n)\Big\}. \tag{2.11}$$

Furthermore, for stability and convergence of the the Godunov scheme (2.9)-(2.11), we consider that the CFL condition: $\lambda \cdot \max\Big\{\big|f'(u)\big| \ : \ u \in I_{\max}\Big\} \leq 1/2$ has to be satisfied.

2.4. **Discrete parameter identification problem.** The continuous observation data $\hat{u}$ are discretized by

$$\hat{u}_j = \frac{1}{\Delta x}\int_{K_j} \hat{u}(x)dx, \quad j = 0, \ldots, M. \tag{2.12}$$

The natural discretization of the parameter identification problem (2.5) is given by

$$\begin{cases} \text{minimize} & \mathscr{J}_\Delta(\mathbf{e}), \qquad \mathscr{J}_\Delta(\mathbf{e}) := \dfrac{1}{2}\displaystyle\sum_{j=0}^{M} |u_j^N(\mathbf{e}) - \hat{u}_j|^2 \Delta x, \\ \text{subject to} & u_j^N(\mathbf{e}) \text{ is obtained by (2.9)-(2.11) for } \mathbf{e} \in D. \end{cases} \tag{2.13}$$

Here, we note that the continous restriction $E\Big(u(\mathbf{e}), p; f(u(\mathbf{e}); \mathbf{e})\Big) = 0$ is replaced by the discrete restriction $u_j^N(\mathbf{e})$ is the numerical solution of (2.1)-(2.3) obtained by the finite volume scheme (2.9)-(2.11). The consistence between the discrete and continuous restrictions is given by the convergence of the monotone finite volume methods.

3. Continuous genetic algorithm for flux estimation

The evolutionary computation techniques imitate the principles of natural selection and evolution. The basis of evolutionary computation are the following four paradigms: genetic algorithms [33], genetic programming [34], evolutionary strategies [35] and evolutionary programming [36]. Of these techniques the genetic algorithms are most popular because of their simplicity of implementation, global convergence property and several other advantages, see [37]. The first genetic algorithm was proposed by Holland in his pioneer work [33]. After this work, several researchers have been developing various improvements. Here, we highlight two important historical points. First, the development of several versions of the original binary genetic algorithms, given by [38]. It was the responsible of wide and rapid diffusion of genetic algorithms. Second, the contributions of Michalewicz and collaborators, mainly the point concerning to real coded genetic algoritms [39]. In contrast, with the classical binary representation of chromosomes, the coding of chromosomes with floating point representation was introduced and proven to have an highly improvements on the implementation, computation speed and precision. A complete review of the state of art of genetic algorithms before 2008 is given by Rocca, Donelli and Massa in [22].

In the sequel, we use the standard terminology of genetic algorithms. For completeness of the presentation we recall the main concepts: chromosomes, gens, population and generation, for further details see [37, 33, 40]. A chromosome is an array of parameters to be identified or where the cost function is evaluated. A gen is a Cartesian coordinate of the parameter set that represents a chromosome (vector). A population is the set of chromosomes. A generation is the population at the end of the one iteration of the genetic algorithm. Furthermore, we recall that genetic algorithms uses several kinds of representation for the chromosomes, being the most wide used the binary representation and the floating-point (real and continuos) representation. In this paper we select a floating-point representation, since the continuous genetic algorithm is inherently faster than the binary genetic algorithm when the cost function is continuous, because the chromosomes do not have to be decoded prior to the evaluation of the cost function. See the books of Haupt-Haupt [40] and Michalewicz [39] for further details on advantages and disadvantages of both representations.

The continuous genetic algorithm implemented in this paper basically consists of two big steps, the selection of the initial population and the natural selection. More specifically we have the following description:

(a) **Initial population**. We define a full matrix that represents a random initial population $\mathbb{E} = \left[\mathbf{e}_1|\mathbf{e}_2|\cdots|\mathbf{e}_n\right]^T$, where each row $\mathbf{e}_j^T \in \Omega := \prod_{i=1}^{d}[l_i, u_i] \subset D \subset \mathbb{R}^d$ with $l_i < u_i$ for $i = 1, \ldots, d$ is a hypercube.

(b) **Natural selection**. Let G be the maximum number of iterations or the maximum number of generations and $q \in \mathbb{Z}_0^+$. Initialize the counter q by $q = 0$ and make the following:

(b1) **Cost of the population.** Define the vector **cost** $\in \mathbb{R}^n$ by evaluation of the cost function on each chromosome of the population $\mathbb{E}$, i.e. $\mathbf{J} := (\mathscr{J}_\Delta(\mathbf{e}_1), \ldots, \mathscr{J}_\Delta(\mathbf{e}_n))^{\mathrm{T}} \in \mathbb{R}^n$, and define the matrix $\hat{\mathbb{E}} = [\mathbb{E}|\mathbf{J}]$. If there is an $\ell \in \{1, \ldots, n\}$ such that $\mathbf{J}_\ell \leq J_{\min}$, then the solution of (2.13) is $\mathbf{e}_\ell$ and the iteration is stopped. Here $J_{\min}$ is an established tolerance for the cost evaluation.

(b2) **Select mates.** We select the parents in three stages. First, we update $\hat{\mathbb{E}}$ by row permutation until the following property $\hat{\mathbb{E}}^q_{1,d+1} \leq \hat{\mathbb{E}}^q_{2,d+1} \leq \ldots \leq \hat{\mathbb{E}}^q_{n,d+1}$ is satisfied. Second, if $s \in (0, 1]$ denotes the selection rate, we select the first $[\![ns]\!]$ rows of $\hat{\mathbb{E}}$ and store the sub-matrix in the so called mating pool matrix $\mathbb{F}$. Here $[\![\cdot]\!]$ is the notation of nearest integer. In the third place, by applying the roulette wheel weighting, we choose the parents from the chromosomes on $\mathbb{F}$.

(b3) **Mating.** We define the algebraic law for the crossover of the parents. In this paper we obtain a offspring by applying a random convex combination of parents gens at the random crossover point. The mating process stops when $n - [\![ns]\!]$ offsprings are generated. Here, in this step, the population matrix $\mathbb{E}$ is updated by considering the parents in the first $[\![ns]\!]$ rows and the offsprings in next ones.

(b4) **Mutation.** If $\mu \in [0, 1]$ denotes the mutation rate, we define the total number of mutations: $m := [\![\mu(n-1)d]\!]$. In this step we repeat m times the following mutation process: the random gen $\mathbb{E}_{ij}$ is replaced by a random number which belongs to the interval $[l_j, u_j]$. We note that after the stop of the mutation the population matrix $\mathbb{E}$ is naturally updated. Set $q = q + 1$ and if $q \leq G$ go to item (b1) else calculate the vector $\mathbf{J}$ and the solution is the chromosome $\mathbf{e}_\ell$ such that $\mathbf{J}_\ell \leq \mathbf{J}_j$ for $j \in \{1, \ldots, n\}$.

The hypercube Ω considered in (a) can be replaced by a convex set such that $\Omega \subset D$. The hypothesis of convexity is needed by the convex combination used in (b3).

4. Numerical results

In this section we consider three example applications of the genetic algorithm used for the flux identification in conservation laws. In all examples the genetic algorithm is run with a population size $n = 20$, selection rate $s = 0.5$ and tolerance $J_{\min} = 1.0 \times 10^{-6}$ for the cost evaluation. The mutation rate for example 1 is set to $\mu = 0.2$ and for examples 2 and 3 to $\mu = 0.37$. The maximum number of iterations for examples 1 and 2 is $\mathsf{iter} = 100$ and for examples 3 is $\mathsf{iter} = 20$. This selection of genetic parameter values is following the suggestions of Haupt and Haupt [40].

On the other hand, the maximum number of time steps in the finite volume method for the three examples are selected via the following relation $N = \left[\!\!\left[T(0.98\Delta x)^{-1} \max_{u \in I_{\max}} |f'(u)| \right]\!\!\right]$, where the interval $I_{\max}$ is detailed in the description of each example.

4.1. Example 1: Identification of a single parameter (d=1).

In this example the flux function in Equation (2.1) is specified to be of Burgers type: $f(u) = u^\alpha/\alpha$, and the initial-boundary conditions are given by

$$u_0(x) = \begin{cases} 0 & \text{for } (4x-1)(4x-3) > 0, \\ 1 & \text{elsewhere,} \end{cases} \qquad \text{and} \quad g_0(t) = g_1(t) = 0 \quad \forall\, t > 0.$$

We note that $f''(u) = (\alpha - 1)u^{\alpha-2}$, which implies that f belongs to the admissible set $\mathscr{U}_{\mathrm{ad}}$ when $\alpha - 1 > 0$, since $I_{\max} = [0, 1]$. Thus, the restriction set in (2.5) is defined as $D = (1, \infty)$.

We take two analytical observations obtained with $\alpha = 2$ at $T_1 = 1/4$ and $T_2 = 1/2$, denoted by $\hat{u}_1$ and $\hat{u}_2$, respectively. By the method of characteristics (see Figure 1) we deduce that $\hat{u}_i : I \to \mathbb{R}$,

for $i = 1, 2$, are defined as follows

$$\hat{u}_1(x) := u(x, 1/4) = \begin{cases} 0, & (4x-1)(8x-7) > 0, \\ 4x-1, & (4x-1)(2x-1) \leq 0, \\ 1, & \text{elsewhere}, \end{cases} \quad \text{and}$$

$$\hat{u}_2(x) := u(x, 1/2) = \begin{cases} 0, & 4x-1 < 0, \\ 2x-1/2, & (4x-1)(4x-3) \leq 0, \\ 1, & \text{elsewhere}. \end{cases}$$

Then, the analytical cost functions are given by

$$\mathscr{J}_1(\alpha) = \frac{1}{8}\left(\frac{\alpha-1}{\alpha+1} - \frac{2(\alpha-1)}{2\alpha-1}\right) + \operatorname{sgn}(\alpha-2)\left(\frac{\alpha-2}{16\alpha}\right) \quad \text{and} \tag{4.1}$$

$$\mathscr{J}_2(\alpha) = \frac{1}{4}\left(\frac{\alpha-1}{\alpha+1} - \frac{2(\alpha-1)}{2\alpha-1} + \frac{1}{3}\right) + (1+\operatorname{sgn}(\alpha-2))\left(\frac{\alpha-2}{16\alpha}\right), \tag{4.2}$$

where sgn is the sign function.

For the genetic algorithm we choose $\Omega = [1.1, 4] \subset D$. The graph of the cost function over Ω is given in Figure 2. In both plots, Figure 2(a) and Figure 2(b), we note that the optimum of the numerical and analytical costs functions does not coincide. This behavior is a natural consequence of the numerical method used for the simulation of the direct problem, since a first order finite volume method comes with a large numerical diffusion, see [29, 31, 32].

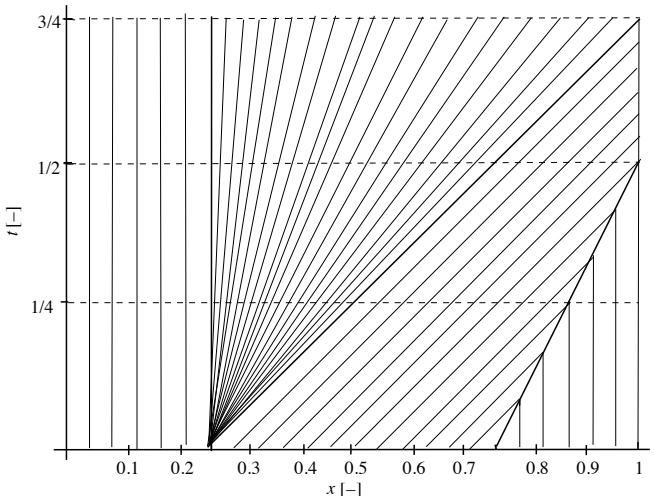


FIGURE 1. Example 1: Configuration of characteristics with $\alpha = 2$.

For the simulation of the direct problem we use $M = 100$ space intervals and choose a variable number of time steps satisfying the CFL condition.

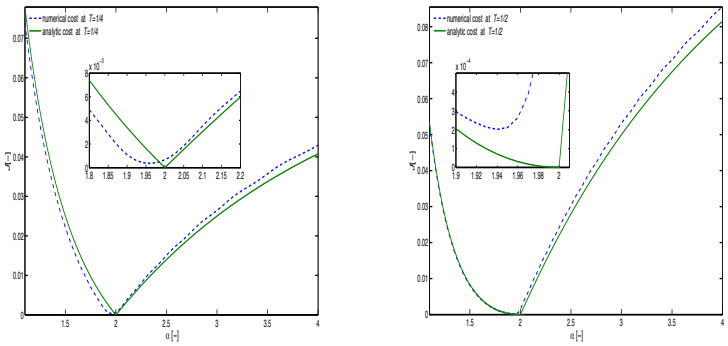
The results of the identification of α are given in Table 1. The best chromosomes of each iteration are given in Table 2. The observed and identified profiles are compared in Figure 3(b) and Figure 3(c). The observed and identified flux functions are compared in Figure 3(d).

From Table 2, we note a fast convergence of the genetic algorithm. The maximum number of generations and the cost tolerance are fixed to 1.0×10^2 and 1.0×10^{-6}, respectively. However, the algorithm found an acceptable extremum within four generations and stops prematurely at 10 generations, when the stopping criteria of cost tolerance is reached.

4.2. **Example 2: Identification of a flux modeling traffic flow (d=2).** We recall that the basic flux function used for traffic flow models is of the following type: $\hat{f}(u) = v_* u\,(1 - u/\rho^*)$, which is a concave function for v_* and ρ^* belongs to $\mathbb{R}^+$, i.e. $\hat{f} \notin U_{\text{ad}}$. It is well known that the analysis of concave flux functions is completely analogous to the case of convex flux functions,

Observation $\hat{u}_1$				Observation $\hat{u}_2$			
Initial population		Final generation		Initial population		Final generation	
α	cost	α	cost	α	cost	α	cost
3.0978	0.02858023	1.9594	0.00036738	2.3049	0.01998901	1.9415	2.01182E-4
1.3222	0.03883032	1.9594	0.00036738	3.3342	0.06547159	1.9415	0.000201182
2.7524	0.02120940	1.9594	0.00036738	1.2853	0.02323202	1.9415	0.000201182
3.4640	0.03503519	1.9593	0.00036739	2.0188	0.00271066	1.9415	0.000201182
1.3758	0.03301540	1.9593	0.00036739	1.2099	0.03258585	1.9415	0.000201182
1.1587	0.06245224	1.9590	0.00036742	2.7299	0.04140269	1.9415	0.000201182
2.7273	0.02055735	1.9590	0.00036742	1.2730	0.02456631	1.9415	0.000201182
3.6778	0.03870158	1.9589	0.00036744	3.9831	0.08510473	1.9414	0.000201183
3.2516	0.03152623	1.9589	0.00036744	2.2301	0.01568804	1.9414	0.000201183
2.8147	0.02276175	1.9589	0.00036744	1.6769	0.00267327	1.9414	0.000201183
2.2748	0.00883104	1.9589	0.00036744	3.3244	0.06508412	1.9414	0.000201183
3.2396	0.03133313	1.9589	0.00036744	1.2958	0.02214488	1.9414	0.000201183
2.2518	0.00808391	1.9589	0.00036744	1.7865	0.00106196	1.9414	0.000201183
1.9375	0.00046090	1.9589	0.00036744	1.6033	0.00441310	1.9414	0.000201183
3.3569	0.03316766	1.9589	0.00036744	2.3370	0.02173338	1.9413	0.000201186
3.6595	0.03844159	1.9589	0.00036744	1.7015	0.00222037	1.9413	0.000201186
3.1396	0.02948630	1.9586	0.00036752	3.0458	0.05484254	1.9879	0.000899494
3.0755	0.02808072	2.7695	0.02165141	3.3520	0.06617539	2.7798	0.043662271
2.7699	0.02166166	3.0405	0.02729970	3.0941	0.05659175	2.8504	0.046921621
2.5272	0.01583049	3.4285	0.03438576	1.5932	0.00470261	3.0967	0.056695360

TABLE 1. Example 1: Evolution of parameter α and cost function value 'cost' for observation $\hat{u}_1$ (left) and $\hat{u}_2$ (right). In both cases, the column denominated 'initial population' shows the 20 initial random chromosomes and their corresponding cost value before the first generation and the column denominated 'final population' shows the 20 chromosomes and their corresponding cost at the 10^{th} generation. For each generation the best individual is marked.



(a) (b)

FIGURE 2. Example 1: (a) The analytical cost function (4.1) (solid line) and the numerical cost function (dotted line), (b) The analytical cost function (4.2) (solid line) and the numerical cost function (dotted line).

q	Observation $\hat{u}_1$		Observation $\hat{u}_2$	
	α	cost	α	cost
0	1.9375	0.00046090	1.7865	0.00106196
1	1.9375	0.00046090	1.9605	0.00026737
2	1.9375	0.00046090	1.9110	0.00025926
3	1.9675	0.00037939	1.9383	0.00020224
4	1.9575	0.00036810	1.9415	0.00020118
5	1.9575	0.00036810	1.9415	0.00020118
6	1.9612	0.00036794	1.9415	0.00020118
7	1.9594	0.00036738	1.9415	0.00020118
8	1.9594	0.00036738	1.9415	0.00020118
9	1.9594	0.00036738	1.9415	0.00020118
10	1.9594	0.00036738	1.9415	0.00020118

TABLE 2. Example 1: The bests chromosomes of the first 11 generations and their corresponding cost function value.

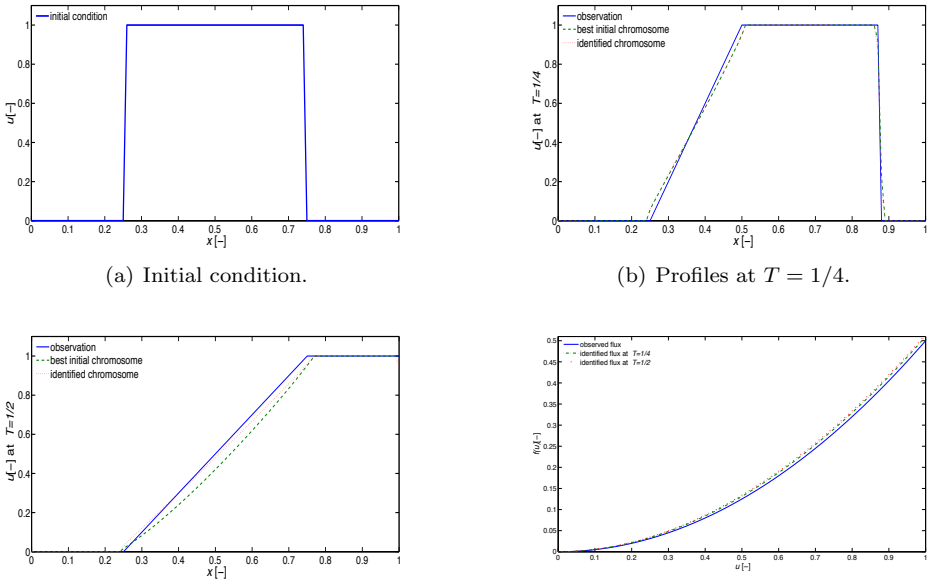
see [15, 29] for details. In this specific case, if we redefine the flux function as follows $\hat{f}_1(u) = -\hat{f}(u) + \hat{f}'(0)u + \hat{f}(0)$, we have that $\hat{f}_1(u) = -v_* u^2/\rho^* \in U_{\text{ad}}$, see [41]. Thus, the analysis of the traffic flow model can be done by following the theory for convex flux functions.

In this example, we consider a slightly more general flux than $\hat{f}_1(u) = -v_* u^2/\rho^*$, namely

$$f(u) = \alpha u^\beta, \quad u_0(x) = \begin{cases} 2, & x \in [0, 1/3), \\ 3, & x \in [1/3, 2/3), \\ 1, & x \in [2/3, 1], \end{cases} \qquad g_0(t) = 0, \quad \text{and} \quad g_1(t) = 1.$$

We note that $f \in \mathscr{U}_{\text{ad}}$ if $\alpha\beta(\beta - 1) > 0$ since $I_{\max} = [0, 3]$. Thus, the restriction set defined in (2.5) is given by

$$D = \Big\{ \mathbf{e} = (\alpha, \beta) \in \mathbb{R}^2 \quad : \quad \alpha\beta(\beta - 1) > 0, \quad f(\cdot; \mathbf{e}) \in \mathscr{U}_{\text{ad}} \Big\}.$$



(a) Initial condition.

(b) Profiles at $T = 1/4$.

(c) Profiles at $T = 1/2$.

(d) Identified and analytical flux.

FIGURE 3. Example 1: (a) The initial condition u_0 for Example 4.1. (b) The random best initial profile at the initial evolution, the identified profile and the analytical profile $\hat{u}_1$ at $T = 1/4$ for Example 4.1. (c) The random best initial profile at the initial evolution, the identified profile and the analytical profile $\hat{u}_2$ at $T = 1/2$ for Example 4.1. (d) Comparison of the flux used for the observation profile and the identified flux. For (b)-(d), see Table 1 for numerical values of best initial and identified parameter.

We consider an analytical observation obtained with $\alpha = 0.25$ and $\beta = 2$ at $T = 1/4$. By the method of characteristics (see Figure 4) we deduce that $\hat{u} : I \to \mathbb{R}$ is defined as

$$\hat{u}(x) \quad := \quad u(x, 1/4) = \begin{cases} 8x, & x(4x-1) \leq 0, \\ 2, & (4x-1)(12x-7) < 0, \\ 8x - 8/3, & (12x-7)(24x-17) \leq 0, \\ 3, & (24x-17)(11x-12) < 0, \\ 1, & (11x-12)(x-1) \leq 0. \end{cases}$$

For the genetic algorithm we choose $\Omega = [0.1, 3] \times [1.1, 4] \subset D$. The graph of the cost function over Ω is shown in Figure 5. The shape of the numerical cost functions for $M = 100$ and $M = 200$ are similar. However, as in the case of Example 1 the numerical diffusion of the Godunov method implies that the extremum for the numerical cost function is slightly different from the extremum of the analytical cost function.

The results of the identification with $M = 100$ and $M = 200$ space steps are given in Table 3. Furthermore, the plot of the profiles is shown in Figure 6.

4.3. **Example 3: Identification of a flux in chromatography (d=3).** Chromatography is a laboratory technique for the separation of mixtures. It can be reasonably modeled by a hyperbolic system governed by nonlinear functions of the mixture concentrations, called isotherm functions, which appears as the flux of the mass-balance equations [42]. In this example, we consider a scalar conservation law with the nonlinear flux modeled by a modified Redlich-Peterson isotherm [43]

$$f(u) = \frac{\alpha u^2}{1 + \sigma u^\beta},$$

$M = 100$						$M = 200$					
Initial population			Final generation			Initial population			Final generation		
α	β	cost	α	β	cost	α	β	cost	α	β	cost
1.7283	3.4338	1.1239	0.1745	2.2739	0.0063	2.6301	3.1473	1.3036	0.3160	1.8248	0.003762
1.5308	3.1295	1.0845	0.1745	2.2739	0.0063	2.3292	3.2303	1.2522	0.3160	1.8248	0.003762
2.9825	1.1012	1.6864	0.1745	2.2739	0.0063	0.5599	3.4016	0.6811	0.3160	1.8248	0.003762
0.1745	1.9267	0.2250	0.1745	2.2739	0.0063	2.6800	3.2769	1.2974	0.3160	1.8248	0.003762
0.8526	1.5953	0.4348	0.1745	2.2739	0.0063	2.3853	2.3041	1.3524	0.3160	1.8248	0.003762
1.0488	1.6894	0.5162	0.1745	2.2739	0.0063	0.6968	2.4075	0.5552	0.3160	1.8248	0.003762
0.4563	1.3746	0.1175	0.1745	2.2739	0.0063	1.8596	3.1455	1.1722	0.3160	1.8248	0.003762
2.2632	1.2122	1.1530	0.1745	2.2603	0.0107	1.4463	3.3838	1.0674	0.3160	1.8248	0.003762
1.9251	2.2407	1.2175	0.1745	2.3092	0.0158	1.0724	3.8551	0.9622	0.3160	1.8248	0.003762
0.6701	1.7770	0.3540	0.1745	2.3670	0.0567	1.4626	2.6769	1.0689	0.3160	1.8248	0.003762
1.4449	1.4266	0.6714	0.1745	2.9074	0.2070	1.2137	1.8713	0.7703	0.3160	1.8676	0.034107
0.8713	2.3571	0.6876	0.1745	3.4616	0.3626	1.1586	2.7404	0.9467	0.3160	3.1048	0.371130
0.1105	1.9181	0.4183	0.1745	3.5301	0.2774	1.5768	3.0794	1.1062	0.3160	3.7089	0.508626
0.4357	3.5786	0.6029	0.1745	3.6887	0.3097	2.1864	3.1035	1.2385	2.1135	1.8248	1.300688
1.7209	1.2010	0.8032	0.1745	3.6890	0.3106	1.4225	2.5499	1.0477	2.2929	1.5230	1.366459
2.6876	3.9489	1.2326	0.1745	1.7517	0.3238	2.8055	2.0329	1.4883	2.4682	1.8248	1.432283
2.7135	3.8700	1.2413	0.1745	3.8098	0.3339	0.8936	3.9869	0.9050	3.3930	1.8248	1.655020
2.1297	3.9547	1.1666	1.1177	2.2739	0.8411	2.5917	3.1348	1.2996	3.6056	1.8248	1.690803
0.7780	3.4745	0.8196	1.9187	2.4159	1.2101	0.1996	1.4223	0.4374	3.6271	1.8248	1.694224
1.6356	1.2255	0.7686	3.9152	2.9713	1.4552	0.8860	2.3507	0.7004	3.7317	1.8248	1.710099

TABLE 3. Example 2: The column labeled $M = 100$ and $M = 200$ show the results at 100 and 200 space steps, respectively. In both cases, the column labeled 'initial population' shows the 20 random chromosomes and their corresponding cost before the first generation and the column labeled 'final population' shows the 20 chromosomes and their corresponding cost at 100^{th} generation. For each generation the best individuals are marked.

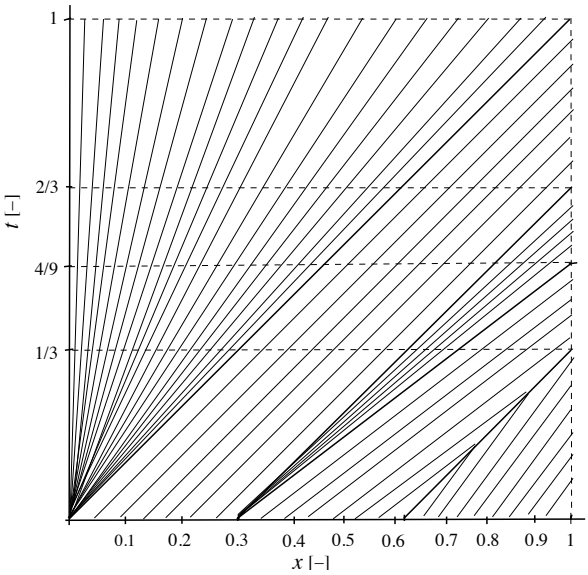


FIGURE 4. Example 2: Characteristics configuration for Example 4.2 with $\alpha = 0.25$ and $\beta = 2$.

where α, σ and β are constant parameters. The identification of the isotherm either of these three parameters α, σ and β from our Redlich-Paterson model, is crucial, from the theoretical point of view, as well as the more practical consideration of accurately governing the experiment to improve separation. In this regard there are several articles in literature on the identification of other isotherms such as Langmuir or Bilangmuir models [7, 8, 16]. We suppose that the initial-boundary conditions are given by

$$u_0(x) = \begin{cases} 0, & (4x-1)(4x-3) > 0, \\ -x^2 + x - 3/16, & \text{elsewhere}, \end{cases}$$

and $g_0(t) = g_1(t) = 0$, respectively. We note that

$$\begin{aligned} f'(u) &= \frac{\alpha u[2 + \sigma(2-\sigma)u^\beta)]}{(1+\sigma u^\beta)^2}, \\ f''(u) &= \frac{\alpha[2 + \sigma(1-\sigma)(4+\beta)u^\beta + \sigma^2(2-\beta)(1-\beta)u^{2\beta}]}{(1+\sigma u^\beta)^3}, \end{aligned}$$

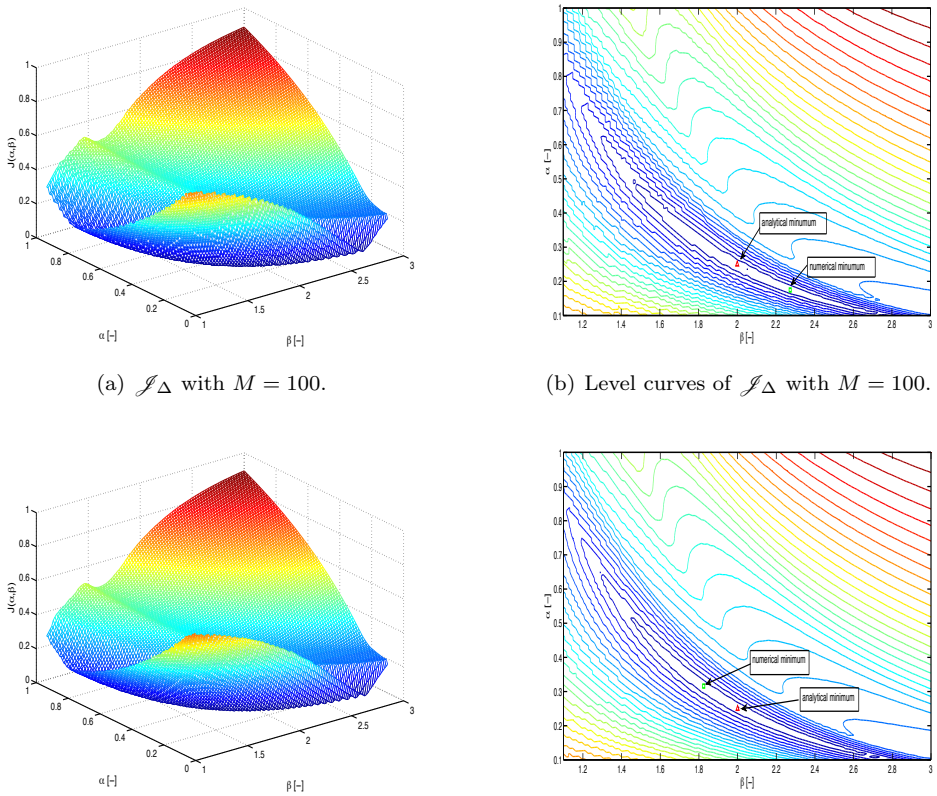
and $I_{\max} = [0, 1/16]$. Consequently, the parameter identification restriction set (2.5) is defined as follows

$$D = \Big\{ \mathbf{e} = (\alpha, \beta, \sigma) \in \mathbb{R}^3 \ : \quad \alpha > 0,\ \beta \in [1,2]\ , \sigma > 0 \text{ and } \quad f(\cdot; \mathbf{e}) \in U_{\text{ad}} \Big\}.$$

The observation data are set as a piecewise linear fit to a simulation of the direct problem with parameters $\alpha = \sigma = 1, \beta = 1.5, M = 500$ and $T = 3$. More precisely, the observation $\hat{u} : I \to \mathbb{R}$ considered for this example is defined as follows

$$\hat{u}(x) = \begin{cases} 0, & x \in [0, 0.25[\cup]0.85, 1], \\ 0.1178x - 0.0288, & x \in [0.25, 0.598], \\ 0.0984x - 0.0174, & x \in]0.598, 0.75], \\ 0.0534x + 0.0168, & x \in]0.75, 0.85]. \end{cases}$$

For the genetic algorithm we choose $\Omega = [0.1, 2] \times [1, 2] \times [0.1, 2] \subset D$. The results of the identification with $M = 200$ space steps are given in Table 4 and the plots of results is shown in Figure 7. The convergence history is given in Table 5 and in Figure 8. We note that the genetic algorithm converged during four generations.



(a) $\mathscr{J}_\Delta$ with $M = 100$.

(b) Level curves of $\mathscr{J}_\Delta$ with $M = 100$.

(c) $\mathscr{J}_\Delta$ with $M = 200$.

(d) Level curves of $\mathscr{J}_\Delta$ with $M = 200$.

FIGURE 5. Example 2: Plots and level curves of discrete cost function $\mathscr{J}_\Delta : \Omega \to \mathbb{R}$ with $M = 100$ (above) and $M = 200$ (below) space intervals.

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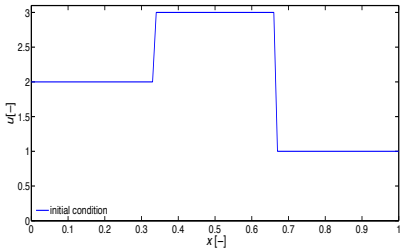
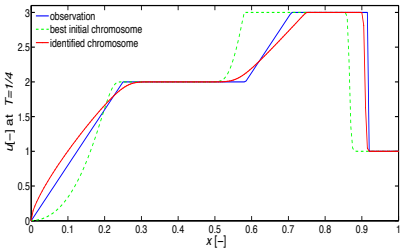
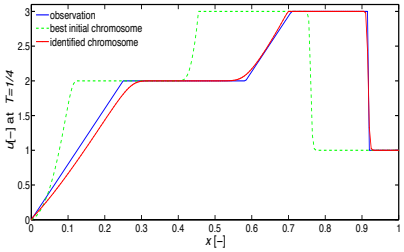


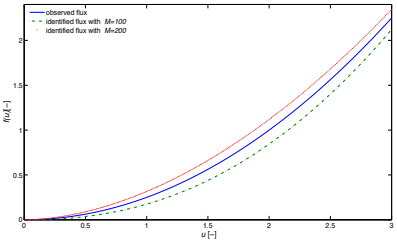
(a) Initial condition.



(b) Results with $M = 100$.

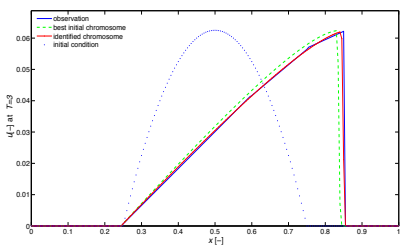


(c) Results with $M = 200$.

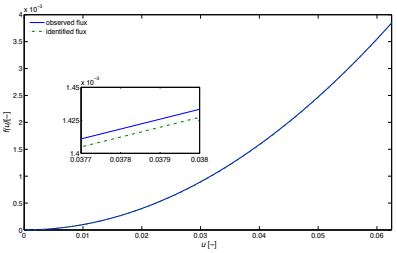


(d) Identified and analytical flux.

FIGURE 6. Example 2: (a) The initial condition u_0 for Example 4.2. (b) The random best initial profile at the initial evolution, the identified profile and the analytical profile $\hat{u}$ at $T = 1/4$ with $M = 100$ for Example 4.2. (c) The random best initial profile at the initial evolution, the identified profile and the analytical profile $\hat{u}_1$ at $T = 1/4$ for with $M = 100$ for Example 4.2. (d) Comparison of the flux used for the observation profile and the identified flux. For (b)-(d), see Table 2 for numerical values of best initial and identified parameter.



(a) Initial condition.



(b) Results with $M = 100$.

FIGURE 7. Example 3: (a) The initial condition u_0, the random best initial profile at the initial evolution, the identified profile and the analytical profile $\hat{u}$ at $T = 3$ for Example 4.3. (b) Comparison of the flux used for the observation profile and the identified flux. See Table 4 for numerical values of best initial and identified parameters.

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Initial population				Final generation			
α	β	σ	cost	α	β	σ	cost
0.9316	1.3251	0.5399	$2.3191E-5$	0.9912	1.7783	0.9433	$1.6432E-7$
0.5911	1.7578	0.3877	$1.5353E-4$	0.9912	1.8513	1.1029	$1.6434E-7$
1.6448	1.1740	0.8284	$1.8691E-4$	0.9912	1.8513	1.1029	$1.6434E-7$
1.2727	1.8093	1.4439	$9.4545E-5$	0.9912	1.8875	0.9433	$2.0864E-7$
0.2460	1.9109	1.4288	$2.7872E-4$	0.9912	1.8513	0.4929	$2.7107E-7$
1.3498	1.7926	1.7633	$1.1675E-4$	0.9912	1.8875	0.5755	$2.9447E-7$
1.8913	1.6329	0.2545	$2.3345E-4$	0.9912	2.1019	0.9433	$2.9722E-7$
0.2823	1.2721	1.1690	$2.6780E-4$	0.9912	1.8513	1.3111	$6.5055E-7$
1.2710	1.8265	0.6863	$9.5575E-5$	0.9912	1.8875	0.2158	$1.0564E-6$
0.7537	1.2150	1.8534	$1.0555E-4$	0.9912	1.7783	1.5167	$1.5097E-6$
1.7066	1.0165	1.4701	$1.8586E-4$	0.9912	1.4546	0.9433	$2.6636E-6$
0.7288	1.8147	1.1011	$9.9594E-5$	0.9751	1.8788	1.2793	$3.5103E-6$
0.2320	1.3725	0.8953	$2.8537E-4$	0.9912	1.2442	0.9433	$8.1190E-6$
0.6477	1.1466	0.3904	$1.3488E-4$	1.1148	0.7222	1.2465	$9.7744E-6$
0.1585	1.0861	1.3607	$3.1185E-4$	0.9341	0.6495	0.9207	$6.5038E-5$
1.8037	1.1925	0.9423	$2.1949E-4$	1.5637	1.7783	1.3346	$1.7336E-4$
1.8683	1.2471	0.9874	$2.3347E-4$	0.9751	0.1082	1.3553	$1.9253E-4$
1.6991	1.0650	1.7788	$1.8445E-4$	0.4825	1.7783	0.6419	$1.9595E-4$
1.3636	1.9357	0.4889	$1.2287E-4$	1.8277	0.9523	0.9020	$2.1762E-4$
1.9712	1.1818	1.7713	$2.4154E-4$	0.2163	1.8513	1.1029	$2.8980E-4$

TABLE 4. Example 3: The initial population columns shows the 20 random chromosomes and their corresponding cost before of the first generation and the final population columns shows the 20 chromosomes and their corresponding cost at 20th. generation. The underline chromosome is the best individual of its generation.

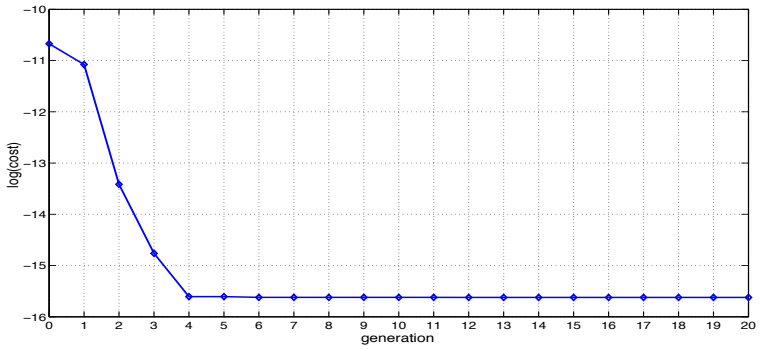

FIGURE 8. Example 3: Convergence history: the generation vs. the better evaluation of cost function, see Table 5 for the numerical value of the chromosomes.

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Generation	α	β	σ	cost
0	0.9316	1.3251	0.5399	$2.3190E-5$
1	0.9911	1.2150	1.5560	$1.5454E-5$
2	0.9911	1.7879	1.5560	$1.4942E-6$
3	0.9911	1.7879	0.5681	$3.8822E-7$
4	0.9911	1.8347	1.1194	$1.6690E-7$
5	0.9911	1.8347	1.1194	$1.6690E-7$
6	0.9912	1.8530	1.1194	$1.6442E-7$
7	0.9912	1.8530	1.1194	$1.6442E-7$
8	0.9912	1.8530	1.1194	$1.6442E-7$
9	0.9912	1.8530	1.1194	$1.6442E-7$
10	0.9912	1.8530	1.1194	$1.6442E-7$
11	0.9912	1.8530	1.1194	$1.6442E-7$
12	0.9912	1.7783	0.9433	$1.6432E-7$
13	0.9912	1.7783	0.9433	$1.6432E-7$
14	0.9912	1.7783	0.9433	$1.6432E-7$
15	0.9912	1.7783	0.9433	$1.6432E-7$
16	0.9912	1.7783	0.9433	$1.6432E-7$
17	0.9912	1.7783	0.9433	$1.6432E-7$
18	0.9912	1.7783	0.9433	$1.6432E-7$
19	0.9912	1.7783	0.9433	$1.6432E-7$
20	0.9912	1.7783	0.9433	$1.6432E-7$

TABLE 5. Example 3: The bests chromosomes of each generation and their corresponding cost, see Figure 8.

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