Kybernetes

Formalism for discrete multidimensional dynamic systems

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FORMALISM FOR DISCRETE MULTIDIMENSIONAL DYNAMIC SYSTEMS

1. Introduction

Some real-life situations are difficult to be modelled using continuous formalisms; they are essentially discrete. On the other hand, some space-time systems need to consider other dimensions. In this paper we introduce a new formalism named as Discrete Multidimensional Dynamic System (DMDS).

The DMDS is useful to model discrete multidimensional systems, i.e., those systems whose state variables depend on a set of independent variables that can include time, space variables, or other determined ones. For instance, if we study the human population pyramid of a country, the state variable will be the country population and the independent variables will be time (evolution) and age (pyramid). In this case, "multidimensional" means "time and age". Another example could be the study of the different species population dynamics of an ecosystem. In this case, the state variables are the different species populations and the independent variables are time (evolution), longitude, latitude and height (space variables). In this case, "multidimensional" means "time, longitude, latitude and height". In addition, the DMDS also states the rigorous definition of state variables and their relationships with the other variables that arise in the formalism, i.e., auxiliary variables and input variables.

The roots of the DMDS must be sought in the formalism provided by Caselles (1994) as a General System Theory. This formalism defines rigorously the state, auxiliary and input variables concepts, as well as their general relationships. Based on Caselles' formalism, the Space-Time Dynamic System (STDS), proposed by Micó and Caselles (1998), is a first attempt to construct models with discrete space-time variation. In fact, a continuous version of the STDS, given for a set of integro-differential equations, was provided by Micó et al. (2008). The DMDS generalises both formalisms, the STDS and its cited continuous version, based on the system formalism stated by Caselles (1994).

The DMDS allows the user to describe the space variation of the state-variables at the same level as time variation and any other possible change-variable and it provides a way to construct concrete models, suitable to solve problems involving time evolution and space distribution of state-variables. For instance, space distribution of population per cohorts (understood "cohort" as "age interval") in a city and its time evolution, or time evolution and space distribution of species belonging to an ecological system.

There are two classical kinds of formal models that introduce the space distribution of the state-variables to describe the dynamics of a system: the *reaction-diffusion model* (Nicolis and Prigogine, 1977), that is typical for open chemical systems, and the *cellular-automata model* (Wolfram, 1994) that tries to represent the states of a system that is distributed inside a set of cells which have a dependence on the neighbour ones. These two models will be explained with more details in Section 3 and compared (formally) with the DMDS. Such comparison demonstrates its compatibility and produces an increase in generality in the DMDS with respect to the other two models, widening the scope of application. Note that the DMDS is a hypothetic-deductive approach. Inductive approaches are based on Statistics and Probability theories and are out of the scope of this work (see for instance Higdon (2002), De Cesare et al. (2001 and 2002) and De Iaco et al. (2002)).

We will apply the DMDS to study the evolution of the population density of an urban system distributed per cohorts and districts. Therefore, there are some problems to deal with: to set up the initial conditions, to validate the model and to present the forecasts provided by the model. Some possible solutions to these problems are detailed in the context of a real case related to the city of Valencia (an important city located in the east of Spain, with approximately 850000 inhabitants). Concretely, the DMDS model has been obtained and validated using data from this city. The evolution of its population density per cohorts and districts under three possible scenarios is forecast with the DMDS model.

The rest of the paper is organized as follows. In order to make the paper self-contained, Section 2 gives some previous definitions, resumes the principal steps needed for the STDS applied in Micó and Caselles (1998), and ends with the definition of the DMDS. Section 3 describes two known approaches for space-time dynamic systems, the reaction-diffusion model (RD) and the cellular automata model (AC), as well as their respective rewriting in terms of DMDS. Section 4 presents the steps needed to build a DMDS.

Section 5 shows an application case by simulating an urban system. Finally, Section 6 is devoted to discussion and presentation of possible future work.

2. Previous definitions and Space-Time Dynamical Systems

For a better understanding of our proposal in relation to previous approaches, some definitions are provided (see Caselles 1993 and 1995 for more formalism details):

- *Input-variable*: **v**ariable that influences other variables and no other variable influences it.
- *Output-variable*: variable receiving influences of other variables.
- *Memory-variable*: variable storing a past value of another variable.
- *State-variable*: **v**ariable that needs a past value of itself to be calculated.

Definition 1. *Change-variables, change-vector and change-space* (Micó et al, 2008).

A variable is a *change-variable* if the state-variables depend on it. We will denote a change variable by $x_i,\ i = 0,1,2,\dots,m$. Then $x_i \in X_i = Rg(x_i)$ where $Rg(x_i)$ is the range of x_i that, generally, is a subset of the real-number set. This concept is equivalent to the concept of “support” used by Klir (1985).

As a consequence, a *change-vector* is: $\vec{r} = (x_0, x_1,\dots, x_m) \in D \subseteq R^{m+1}$, where $D = X_0 \times X_1 \times \cdots \times X_m$ is the *change-space*.

Definition 2. *Accessibility domain for change-vectors* (Micó et al, 2008).

Given a STDS, the change space D and a vector $\vec{r} \in D$, we define the *accessibility domain* **of** $\vec{r}$ as the subset of vectors $\vec{r}\,' \in D$ such that there exists at least a state-variable V_{i_0} with $V_{i_0}(\vec{r})$ depending on $\vec{r}\,'$ explicitly or implicitly through state or input-variables. The accessibility domain for $\vec{r}$ will be denoted as $AD(\vec{r})$.

Given $\vec{r} \in D$ and $x_i,\ i = 0,1,\dots,m$ a component of $\vec{r}$, the *accessibility domain* for this component is defined in a similar way, as $AD(x_i|\vec{r}) = \{x_i' : \vec{r}\,' = \{x_0', x_1',\dots, x_m'\} \in AD(\vec{r})\}$.

Observe that if a value of the time variable, $x_0 = t$ is considered, its accessibility domain must be included, by definition, in the set $\{t' \in T = X_0 : t' \leq t\}$ because dependencies between variables cannot exist in later time instants than those being calculated.

Next, we resume the principal steps needed for the Space Time Dynamical Systems (STDS) applied in (Micó and Caselles, 1998):

Step 1. Assume that the system has a space support with volume V. Such space support is divided into M cubes or cells, which represent important space parts in the system, for instance, districts in cities, regions in countries, etc. These cubes can be distributed in three dimensions such as longitude, latitude and height. These cells or space parts of the system are numbered with a set of three integer indexes: (p,q,r) *where* $p \in \{1,2,\ldots,P\}$; $q \in \{1,2,\ldots,Q\}$; $r \in \{1,2,\ldots,R\}$;and $M = P \cdot Q \cdot R$. Thus, the state-variables are characterised by four coordinates, $V_i(n;p,q,r)$, where $n = 0,1,2,\ldots,$ is the considered time instant.

Step 2. State that time evolution of each variable in each cube is due to the following causes:

i. Relationships between variables in each cube, which represent the internal dynamics in each one of them. That is,

$$V_i(n+1;p,q,r) = V_i(n;p,q,r) + F_i^{n \to n+1}(\vec{V}(n;p,q,r), \vec{X}(n;p,q,r))$$

depends on a function $F_i^{n \to n+1}(\vec{V}(n;p,q,r), \vec{X}(n;p,q,r))$ that represents the time change between $t = n$ and $t = n+1$ of state-variables in each cell (p,q,r). Functions F_i depend on a vector of state-variables $\vec{V}(n;p,q,r)$, and on a vector of input-variables $\vec{X}(n;p,q,r)$ From now on functions F_i will be named as *time-rates*.

ii. Relationships between variables in different cells, or *diffusions* between cells. That is, time change of state-variables in a cell (p,q,r) can be due to entrance of state-variables (input diffusion) coming from other cells (for instance, population immigration to a district of a city coming from other districts), and exit of state-variables (output diffusion) towards other cells (for instance, population emigration from a district of a city going to other districts).

Following this idea, consider two different cells, $(p,q,r) \neq (p',q',r')$. Then, *the input diffusion* (*ID*) of state-variable V_i to (p,q,r) coming from (p',q',r') between time instants $t = n$ and $t = n+1$ will be represented by $ID_i^{n \to n+1}((p,q,r) \leftarrow (p',q',r'))$, and the *output diffusion* (*OD*) of state-variable V_i from (p,q,r) towards (p',q',r') between time instants $t = n$ and $t = n+1$ will be represented by $OD_i^{n \to n+1}((p,q,r) \to (p',q',r'))$.

Both, input and output diffusions represent the dynamics between different cells in the system. Consequently:

$$\begin{aligned} V_i(n+1;\vec{m}) &= V_i(n;\vec{m}) + \\ &+ F_i^{n \to n+1}(\vec{V}(n;\vec{m}), \vec{X}(n;\vec{m}) + \\ &+ \sum_{m' \neq m} ID_i^{n \to n+1}(\vec{m} \leftarrow \vec{m}') - \\ &- \sum_{m' \neq m} OD_i^{n \to n+1}(\vec{m} \to \vec{m}') \end{aligned} \quad \text{(Eq.2.1)}$$

where all possibilities of input and output diffusions are added and, to simplify, vectors $\vec{m} = (p,q,r)$ and $\vec{m}' = (p',q',r')$ are defined.

Let $BD_i^{n \to n+1}(\vec{m}, \vec{m}')$ be the *balance diffusion* (*BD*) rates, defined for $i = 1,2,\ldots,h$, as:

$$BD_i^{n \to n+1}(\vec{m}, \vec{m}') = ID_i^{n \to n+1}(\vec{m} \leftarrow \vec{m}') - OD_i^{n \to n+1}(\vec{m} \to \vec{m}')$$

Then, Eq.2.1 can be finally rewritten as:

$$\begin{aligned} V_i(n+1;\vec{m}) &= V_i(n;\vec{m}) + \\ &+ F_i^{n \to n+1}(\vec{V}(n;\vec{m}), \vec{X}(n;\vec{m})) + \\ &+ \sum_{m' \neq m} BD_i^{n \to n+1}(\vec{m}, \vec{m}') \end{aligned} \quad \text{(Eq.2.2)}$$

A necessary remark must be done when output diffusion from $\vec{m} = (p,q,r)$ to $\vec{m}' = (p',q',r')$ is the same than the input diffusion to $\vec{m}' = (p',q',r')$ from $\vec{m} = (p,q,r)$, then only input diffusion rates are needed to be evaluated. In this case:

$$BD_i^{n \to n+1}(\vec{m}, \vec{m}') = ID_i^{n \to n+1}(\vec{m} \leftarrow \vec{m}') - ID_i^{n \to n+1}(\vec{m}' \leftarrow \vec{m})$$

Note that both balance diffusion rates between two different cells depend on state-variables and input-variables, that is:

$$BD_i^{n\to n+1}(\vec{m},\vec{m}') = G_i^{n\to n+1}(\vec{V}(n,\vec{m}),\vec{V}(n,\vec{m}'),\vec{X}(n,\vec{m}),\vec{X}(n,\vec{m}')),\quad i=1,2,\ldots,h \text{ (Eq.2.3)}$$

In order to find out the form of these dependencies we formulate the hypothesis about their mathematical structure by defining some suitable auxiliary-variables for disaggregating model (if necessary) or by fitting some linear or nonlinear functions.

By using Definition 2, the STDS can be extended to:

$$\vec{V}(\vec{r}) = \vec{H}(\vec{V}(AD(\vec{r})), \vec{X}(AD(\vec{r})), AD(\vec{r})) \qquad \text{(Eq.2.4)}$$

This equation has been called DMDS. Note that in the particular case of the STDS, Eq.2.2, the vector function $\vec{H}$ is the addition of the state-variables vector for $\vec{r}$ (changing *n+1* for *n* in its first component) plus the time rates and the space-time rates.

The accessibility domain of the time variable, allows stating the next definitions:

Definition 3.*Memory of a System.*

Given the DMDS and for each $\vec{r} = (t^{\vec{r}}, x_1^{\vec{r}},..., x_m^{\vec{r}}) \in D$, let $AD(t^{\vec{r}}|\vec{r}) = \{\{t_j^{\vec{r}}\}_{j=1}^{p(\vec{r})} : t_j^{\vec{r}} < t_{j+1}^{\vec{r}} \le t^{\vec{r}}, j = 1,..., p(\vec{r})-1\}$ be the accessibility domain for its first component, the memory of the system is defined as the natural number $\max_{\vec{r}\in D}\{t^{\vec{r}} - t_1^{\vec{r}}\}$.

Similarly, a kind of "memory" for the other change variables is defined as follows:

Definition 4.*Reach for each change variable.*

Given the DMDS, and for each $\vec{r} = (t^{\vec{r}}, x_1^{\vec{r}},..., x_m^{\vec{r}}) \in D$ let $AD(x_i^{\vec{r}}|\vec{r})$ be the accessibility domain for the component *i* of $\vec{r}$ $(i = 0,\ldots,m)$. The *reach for each change variable* x_i is defined as the number

$r_i = \max_{\vec{r} \in D} \left\{ \left| x_i^{\vec{r}} - x_i' \right| : x_i' \in AD(x_i^{\vec{r}} | \vec{r}) \right\}$. It is evident that the reach for the time variable (r_0) is equivalent to the memory of the system.

3. Previous approaches to space-time dynamical systems

In this section,two major previous approaches (historically speaking) for space-time dynamic descriptions of systems will be discussed as well as their relation with our DMDS approach.

3.1. The *reaction-diffusion* approach

A reaction-diffusion model for an open chemical system (Nicolis and Prigogine, 1977) tries to describe time evolution and space distribution of several chemical components reacting between them, constituting a system with constant volume that can exchange material of some of its components with its environment. It can be written as:

$$\frac{\partial \rho_i}{\partial t} = F_i(\vec{\rho}) + \vec{\nabla} \cdot \vec{J}_i(\vec{\rho}); \quad i=1,2,...,h \text{ (Eq.3.1.1)}$$

where ρ_i and $J_i(\vec{\rho})$ $(i=1,2,...,h)$ are, respectively, partial densities of chemical components, and spatial density rates. Functions F_i inform about time change of each component in each infinitesimal volume in the system, per unit of volume, given by the "Action Mass Law" for chemical reactions. Vector functions J_i give the rate of cross-change perpendicularly taken to the surfaces of infinitesimal volume components, per unit of surface and volume, in the three spatial directions.

If in Eq.3.1.1 the hypothesis that $\vec{J}_i(\vec{\rho}) = D_i \vec{\nabla} \rho_i$ is stated, equation that is known as the Fick Law, where D_i represent the diffusion coefficients and are constants, then:

$$\frac{\partial \rho_i}{\partial t} = F_i(\vec{\rho}) + D_i \cdot \nabla^2 \rho_i; \quad i=1,2,...,h \qquad \text{(Eq.3.1.2.)}$$

Equation 3.1.2 can be converted in a system of equations with finite differences, by using the same notation than Eq. 2.1, such as:

$$\begin{aligned}
&\rho_i(t+Dt;\vec{m}) = \rho_i(n;\vec{m}) + \\
&+Dt \cdot F_i^{t\to t+Dt}(\vec{V}(t;\vec{m}), X(n,\vec{m}) + \\
&+\frac{Dt}{Dl} \cdot \sum_{m'\neq m} J_i^{t\to t+Dt}(\vec{m} \leftarrow \vec{m}') - \qquad \text{(Eq.3.1.3.)} \\
&-\frac{Dt}{Dl} \cdot \sum_{m'\neq m} J_i^{t\to t+Dt}(\vec{m} \to \vec{m}')
\end{aligned}$$

where $\vec{m} = (x, y, z)$; $\vec{m}' \in \{(x \pm Dx, y, z), (x, y \pm Dy, z), (x, y, z \pm Dz)\}$; with $Dl=Dx=Dy=Dz$. If continuous values are replaced by integer ones, then: $\vec{m} = (p, q, r)$, $\vec{m}' = (p', q', r')$, $\vec{m}' = \{(p \pm 1, q, r), (p, q \pm 1, r), (p, q, r \pm 1)\}$, *Dt=Dl=1*, and Eq.3.1.3 is converted in Eq.3.1.4:

$$\begin{aligned}
&\rho_i(n+1;\vec{m}) = \rho_i(n;\vec{m}) + \\
&+Dt \cdot F_i^{n\to n+1}(\vec{V}(n;\vec{m}), X(n,\vec{m})) + \\
&+\frac{Dt}{Dl} \cdot \sum_{m'\neq m} J_i^{n\to n+1}(\vec{m} \leftarrow \vec{m}') - \qquad \text{(Eq. 3.1.4)} \\
&-\frac{Dt}{Dl} \cdot \sum_{m'\neq m} J_i^{n\to n+1}(\vec{m} \to \vec{m}')
\end{aligned}$$

Note that no space-rates are defined between no-neighbour cells. That is because the *reach* (Definition 4) for the three space change variables is *one* and, even between neighbour cells, Eq. 3.1.4 does not consider the relationships between cells with more than one different coordinate.

The DMDS, or its particular case the STDS, has eliminated these last restrictions. There, all necessary space rates between cells are present. Formally, the reach for both change-space variables can be the maximum possible, so all cells of the system can be put into a relationship. Therefore, these proposed models can be considered as a generalisation of the reaction-diffusion models in their finite differences form.

3.2. The *cellular-automata* approach.

A *cellular-automaton* (Wolfram, 1994) is given by a space-time distribution of a collection of automata or *cells* whose states can be described by a magnitude *V*. That is:

$$V_i(t+1;\vec{m}) = H_i(t;\{\vec{m}'\}) \qquad \text{(Eq.3.2.1)}$$

where $\vec{m} = (p,q,r)$ $(p = 1,2,\ldots,P; q = 1,2,\ldots,Q)$, represents the position of a cell in space and $\{\vec{m}'\}$ is the set of adjacent cells that are near the cell occupying the given position. Generally, the procedure to work with this kind of models consists of formulating some general hypothesis about function *H*and studying the quantitative and qualitative behaviour of the model that includes such hypothesis. Nevertheless, this strategy can be improved in order to model a complex system. Transforming Eq.3.2.1 in the following way:

Firstly, extend the set $\{\vec{m}'\}$ to all cells such that $\vec{m}' \neq \vec{m}$ and, finally, separate the dependence on $\vec{m}$ cell from the dependence between different cells, similarly to Eq.2.1, that is:

$$\begin{aligned} & V_i(t+1;\vec{m}) = H_i(t;\{\vec{m}'\}) = \\ & = F_i(\vec{V}(t;\vec{m}), X(t;\vec{m}) + \\ & + G_i(\vec{V}(t;\vec{m}), \vec{V}(t;\vec{m}'), \vec{X}(t;\vec{m}), \vec{X}(t,\vec{m}')) \end{aligned} \qquad \text{(Eq.3.2.2)}$$

If time is considered asan integer, $t = n,$ functions F and G are considered as rates between $t = n$ and $t = n+1$ and, the number of state-variables increase in $h \geq 1$, then:

$$\begin{aligned} & V_i(n+1;\vec{m}) = H_i(n;\{\vec{m}'\}) = \\ & = F_i^{n \to n+1}(\vec{V}(n;\vec{m}), \vec{X}(n;\vec{m}) + \\ & + G_i^{n \to n+1}(\vec{V}(n;\vec{m}), \vec{V}(n;\vec{m}'), \vec{X}(n;\vec{m}), \vec{X}(n;\vec{m}')), \quad i = 1,2,\ldots,h. \end{aligned} \qquad \text{(Eq.3.2.3)}$$

Eq.3.2.3 should be the same than Eq.2.2if Eq.2.3 is taken into account. These equations are, basically, the same STDS.

Observe that the reach for change-space variables depends on the particular model, but generally do not reach to all the set of cells. On the other hand, the number of state-variables is only one and, in most of the cases, more than one state-variable are needed for describing a complex system.

4. Steps for building a DMDS

The DMDSmodel is an adaptation of the steps suggested by Caselles (1994) with the purpose of constructing models of systems with multidimensional variation. Once the relevant variables are found, the functional relations between the variables can be obtained by following the next steps:

Step 1: Determination of all state-variables that are going to describe formally the real system $V_1, V_2, ..., V_h$. These variables must describe the basic information about the goal stated for the model.

Step 2: Statement of all change-variables that state-variables depend on, including the time-variable. If $\vec{r} = (t, x_1, ..., x_m)$ is the change-vector that contains all of them, then the state-variables can be defined as the scalar fields $V_1(\vec{r}), V_2(\vec{r}), ..., V_h(\vec{r})$.

Step 3: Setting up the hypothesis about the accessibility domain of each change-variable. Implicitly, it is assumed that a model type Eq.2.4is required.

Step 4: Finding the functional relationships between the state-variables V_i at each vector-value $\vec{r}$ and the same and other variables at the vector-values $\vec{r}\,'$ belonging to the accessibility domain of $\vec{r}$.

That is, looking for the functions H_i, components of $\vec{H}$, ofEq.2.4. Such functions can include auxiliary and input-variables(for instance, they can include regression relationships obtained from databases).

Step 5: Validation of the built model, maybe by comparing its results with the historical values of the state-variables, taking into account the initial conditions for the state-variables and the historical values of the input-variables. In order to perform the validation of a DMDS by this instance method, the following procedure is proposed.

Let $U_i(t_j, \vec{m})$, with $i = 1,2,\ldots,h,\ j = 1,2,\ldots,s,$ be the historical values for the state-variables at t_j time instants and at vector-values: $\vec{m} \in Rg(x_1) \times Rg(x_2) \times \cdots Rg(x_m)$. On the other hand, let $V_i(t_j, \vec{m})$ be the predicted values for the state-variables at the same time instants and vector-values. Thus, for each time instant t_j, a degree of fitting between both sets of values can be defined as the determination coefficient:

$$R_i^2(t_j) = \frac{\sum_{\vec{m}} \left(V_i(t_j,\vec{m}) - E\left(U_i(t_j,\vec{m})\right)\right)^2}{\sum_{\vec{m}} \left(U_i(t_j,\vec{m}) - E\left(U_i(t_j,\vec{m})\right)\right)^2}$$

where $E(\cdot)$ means the average value.

Another possible validation method consists of performing a comparison with other models (Sargent, 1999). In this paper, such comparison is performed theoretically (see Section 3) with Reaction-Diffusion models and with Cellular-Automata models and practically (see Section 5) with Reaction-Diffusion models inside an application case.

Step 6: Using the validated model to find, for the adequate simulations, the best values for input-variables in order to reach the goal of the model.

5. Application of a DMDS model to study the population dynamics of an urban system

The following application case is presented in order to demonstrate how the DMDS could be used in a possible real life problem: to obtain a space-time model (the *city model* in the following) of the demographic evolution of an urban system.

The role of the reaction-diffusion models and the cellular-automata models to model the space-time dynamics of urban systems have been very important. For instance, Zannette&Manrubia (1997) use areaction-diffusion model to study the dynamics of a city formation, while Kolokonikov et al. (2012) study the evolution of urban crime by using also a reaction-diffusion model. On the other hand, White & Engelen (1993) use a cellular-automata model to study the evolution of the urban land-use patterns, while Couclelis (1997) uses the geographic information systems to construct a cellular-automata model to study the urban and regional dynamics.

A first primitive space-time demographic model was presented by Micó and Caselles (1998), being its main objective to determine the evolution of the population of a city by districts and cohorts. On its forecasts the city could base its public health, schooling and policies about social services. The main features of this model are the following: (a) it has a single state variable, the corresponding to population per cohorts and districts; (b) the migration rate between districts is computed, as a working hypothesis, as directly proportional to the population of the input district and inversely proportional to the population of the output district and to the distance between districts. The predictions of this model provide some unstable solutions that do not correspond with the real evolution of the system.

In this paper, in order to improve such predictions, a new space-time demographic model is constructed, considering that the state-variable is population density - and not population - per cohorts and districts. On the other hand, the migration rate between districts is computed as a function of the product between the population of the input and the output districts and the difference between both populations (see Equation 5.2). The present model is better than its predecessor because it has been validated through the determination coefficient corresponding to the year 2001. Let us present this model following the steps described in Section 4.

5.1. Steps to build the DMDS corresponding to the *city model*

Step 1. The list of variables found for this model is:

- Input-variables:

  NUCO: number of cohorts. **NUDX**: number of longitude steps. **NUDY**: number of latitude steps. **TNAC**: birth rate ($^0/_{00}$). **TDIF**: migration rate between districts (cells). **XACO(NUCO-1)**: number of years of each cohort except the last one. **TDEF(NUCO):** death rate ($^0/_{00}$). **SMIG**: migratory balance. **DDDT**: Time increment (years). **DDXY**: Area of each district (step^2) .

- State-variable:

  POBI(NUCO,NUDX,NUDY): initial population density per cohorts and districts.**POBL(NUCO,NUDX,NUDY):** present population density per cohorts and districts.

- Auxiliary variables:

CFMI(NUCO): composition of families per cohorts (values between 0 and 1). **CREC(NUCO,NUDX,NUDY):** births and growing rates per cohorts and districts. **DEFU(NUCO,NUDX,NUDY)**: deaths per cohorts and districts.

POBT: total population at the beginning of each year. **POBF(NUCO)**: total population per cohorts. **XMIG(NUCO,NUDX,NUDY)**: migratory balance per cohorts and districts. **POBA(NUDX,NUDY)**: total population per districts. **DIFE(NUCO,NUDX,NUDY,NUDX,NUDY):** balance diffusion rate of population between districts per cohorts.

Note that variable's names followed by other ones in brackets are arrays and represents the range of the change-variables except time, which is not included because the equations are written in visual BASIC, in such a way that the intelligent system SIGEM (Caselles, 1994, 1996) can update the values of each output-variable at each time-step by using the memory-variables (POBI, for this model). Therefore it is not necessary to include time there.

Step 2. The change-variables are time (*t*), cohorts of the population (*i*), and latitude and longitude (respectively, *j* and *k*). Thus, the change-vector is $\vec{r} = (t,i,j,k)$. To simplify the equations, vector $\vec{m} = (i,j,k)$ is used inside some of them. For instance, $\vec{r} = (t,\vec{m})$.

Their respective ranges are $Rg(t) = N$ (natural numbers) for time-variable, $Rg(i) = \{1,2,...,NUCO\}$ for cohorts, $Rg(j) = \{1,2,...,NUDX\}$ for longitude, $Rg(k) = \{1,2,...,NUDY\}$ for latitude. Therefore, the change-space is $D = N \times Rg(i) \times Rg(j) \times Rg(k)$. In order to make possible to define cohorts of different range, the variable *XACO(NUCO-1)* or a number of years of each cohort except the last one, is introduced as an input-variable.

Step 3. The hypothesis about accessibility domains of change variables are:

- For time-variable $AD(t|\vec{r}) = \{t - dt\} \ \forall \ \vec{r} \in D$; thus, the memory of the system is one.

- $AD(i|\vec{r})$ depends on the value of *i*, so, $AD(1|\vec{r}) = Rg(i)$ because the first cohort incorporates the births, and the births depend on the entire population (the sum of all cohorts of population, POBA); $AD(i|\vec{r}) = \{i-1\}$ if $1 < i < NUCO$ and $AD(NUCO|\vec{r}) = \{NUCO-1, NUCO-2\}$ (see equations below).
- $AD(j|\vec{r}) = Rg(j)$ and $AD(k|\vec{r}) = Rg(k)\ \forall \vec{r} \in D$; thus, the reaches of space-change-variables are NUDX and NUDY, respectively. That means that every district of the city can be related with every other one.

Step 4. The functional relationships between the state-variables V_i at vector-values $\vec{r}$ and $\vec{r}'$ such that $AD(\vec{r}) = \{\vec{r}'\} \subseteq D$, are given by the following equations (some of them explained afterwards):

1. POBL :

$$\begin{cases} pobl(t,\vec{m}) = pobi(t,\vec{m}) + \frac{dddt}{ddxy}(crec(t,i,j,k) - crec(t,i+1,j,k) - defu(t,\vec{m}) + xmig(t,\vec{m}) + \\ \quad + \sum_{(j',k')\neq(j,k)} dife((i,j,k),(i,j',k')); \qquad \text{if } i < \text{nuco} \\ pobl(t,\vec{m}) = pobi(t,\vec{m}) + \frac{dddt}{ddxy}(crec(t,i,j,k) - defu(t,\vec{m}) + xmig(t,\vec{m}) + \\ \quad \sum_{(j',k')\neq(j,k)} dife((i,j,k),(i,j',k')) \qquad \text{if } i = \text{nuco} \end{cases}$$

2. POBI: $pobi(t + dddt, \vec{m}) = pobl(t, \vec{m})$

3. CREC:

If i=1 (births): $crec(t,1,j,k) = poba(t,j,k)\frac{tnac}{1000}$

If 1<i<nuco:

$$\begin{cases} crec(t,\vec{m}) = \left(\frac{pobi(t,i,j,k)}{xaco(i)} - \frac{pobi(t,i-1,j,k)}{xaco(i-1)}\right) \cdot \frac{xaco(i-1)}{xaco(i-1)+xaco(i)} ddxy + \\ \frac{pobi(t,i-1,j,k)}{xaco(i-1)} ddxy \end{cases}$$

If $i = nuco$:

$$\begin{cases} crec(t,\vec{m}) = \left(\frac{pobi(t,nuco-1,j,k)}{xaco(nuco-1)} - \frac{pobi(t,nuco-2,j,k)}{xaco(nuco-2)}\right) \cdot \frac{xaco(nuco-1)\cdot ddxy}{xaco(nuco-2)+xaco(nuco-1)} + \\ \frac{pobi(t,nuco-1,j,k)}{xaco(nuco-1)} \cdot ddxy \end{cases}$$

If $crec(t,\vec{m}) < 0$ **:** $crec(t,\vec{m}) = 0$

If xaco(i-1)<1.5: $crec(t,\vec{m}) = pobi(t,i-1,j,k)) \cdot ddxy$

4. DEFU: $defu(t,\vec{m}) = pobi(t,\vec{m})\dfrac{tdef(i)}{1000}\cdot ddxy$

5. XMIG: $xmig(t,\vec{m}) = smig \cdot cfmi(t,i)\dfrac{poba(t,j,k)}{pobt(t)}$

6. DIFE: *If* $poba(t,j',k') = poba(t,j,k)$ or (j=j' and k=k'): $dife((i,j,k),(i,j',k')) = 0$

else $dife((i,j,k),(i,j',k')) = tdif\,\dfrac{(poba(t,j',k')\cdot poba(t,j,k))\cdot cfmi}{\sqrt{(j-j')^2+(k-k')^2}}$

7. POBA: $poba\ (t,j,k) = ddxy\ \cdot \sum_{i} pobi\ (t,\vec{m})$

If $poba(t,j,k) \le 0$: $poba\ (t,j,k) = 1$

8. POBT: $pobt\ (t) = ddxy \cdot \sum_{\vec{m}} pobi\ (t,\vec{m})$

9. CFMI: $cfmi(t,i) = \dfrac{pobf(t,i)}{pobt(t)}$

10. POBF: $pobf(t,i) = ddxy\cdot \sum_{(j,k)} pobi(t,i,j,k)$

Step 5 In order to validatethe DMDS given by the *city model*, its equations have been written in visual BASIC, as required by the intelligent system SIGEM (Caselles, 1994, 2008), and a simulator for the situation has been built. This validation has been performed using the historical data taken from Valencia-city in Spain, during the period 1996-2001, choosing the initial conditions in 1996. For this concrete case and for this period, the values for input-variables have been obtained in the official statistical data-base of the city (http://www.ayto-valencia.es). Details are presented in Section 5.3 and results are shown in Figure 1.

Step 6. Some instance simulations performed with the validated model are presented in Section 5.3.3.

Remarks:

- Observing its equations, it can be deduced that the memory of the model is one and the reach of the other change-variables is the maximum possible. Observe also that POBI is the memory-variable, needed to define the state-variable POBL.
- This last idea - the reaches of the change-variables are the maximum possible - provides the degree of interrelation between space parts inside the system and could be considered, hypothetically, as a common feature for social and socioeconomic systems.

- Observe that the time-rates are computed through the auxiliary-variables CREC, DEFU and XMIG, and the space-rate is computed through the auxiliary-variable DIFE; the state-variable is POBL; the input-variables are SMIG, TDIF, TDEF, TNAC, XACO, DDDT and DDXY, the auxiliary-variables are POBA, POBT, CFMI and POBF; and POBI is the memory variable.
- The strategy to reach these equations was, firstly, to find a valid model of the city without considering space and, finally, to introduce space-rates by following the ideas given by Eq.2.1.
- The equations leading to calculate CREC are based on the following assumptions:
  - The number (NUCO) and length (XACO) of the population-cohorts to be considered are input-variables. That is, the model is able to be adapted to different situations.
  - The transition rates between adjacent cohorts (CREC) are calculated by smoothing linearly the corresponding step.
- The initial values of population density (POBI) and the diffusion rates (DIFE) are estimated or calculated as specified in Sections 5.1.1 and 5.1.2.

5.1.1 Obtaining the initial values of population density (POBI)

The values for POBI corresponding to years 1998, 1999 and 2001 do not exist in historical records. In order to estimate such values, an interpolating polynomial fitted to the data corresponding to years 1991, 1996 and 2001 hasbeen used.

The values of POBI in 1996, for $NUCO \cdot NUDX \cdot NUDY = 2370$ points are unknown but, nevertheless, such values measured as inhabitants/hectare per districts, and the longitudes and latitudes corresponding to the centre of gravity of each district are known in 1996 and in 2001 (the values corresponding to this last year are used latter in order to validate the model by comparing them with the predicted ones). Longitudes and latitudes are assigned, respectively, starting from the western and southern boundaries of the city (longitude one and latitude one, respectively) up to the eastern and northern ones (longitude seventy-nine and latitude ten, respectively). In addition, each point represents an area of 4.594 hectares (the value of DDXY). The population density per cohorts for every pair longitude-latitude belonging to the specified range has been calculated as follows:

1. To perform a linear interpolation using the data of population density and the equation of the plane determined by the closest three points to each point for which the population density must be calculated.
2. To multiply each calculated density by the corresponding global proportion of each cohort in Valencia, in 1996. Due to three cohorts have been considered (NUCO = 3 in simulations), such proportions are 0.141, 0.698 and 0.161, respectively.

The determination coefficients (R^2) corresponding to the three cohorts of population density (2001) (between 0 and 1) are 0.993374, 0.995262 and 0.947411 respectively.

5.1.2 Calculating the diffusion rates (DIFE)

Let $id((j,k) \leftarrow (j',k'))$ be the *input population diffusion* to cell *(j,k)* coming from cell *(j',k')*. The aim of this second step was to find the best dependence of this variable on *poba(j,k)*, *poba(j',k')* and longitudes (*j and j'*) and latitudes (*k and k'*), by using the fitting functions finder REGINT (Caselles, 1998). After some preliminary tests, and using the data obtained as it has been described in Section 5.1.1, the best dependence found was the following function of the populations of the input and output districts and of the distance between them:

$$id((j,k) \leftarrow (j',k')) = a + b \cdot \frac{(poba(t,j',k') \cdot poba(t,j,k))}{\sqrt{(j-j')^2 + (k-k')^2}} + c \cdot \frac{(poba(t,j',k') \cdot poba(t,j,k))}{poba(t,j',k') - poba(t,j,k)} \quad \text{(Eq. 5.1)}$$

Eq. 5.1 has been fitted to the data from the three years: 1998, 1999 and 2000 and a determination coefficient ($R^2 = 0.93$) has been obtained. This is a very acceptable value in order to use Eq. 5.1 inside the model. The average values for parameters *a*, *b* and *c*, computed from the three equations corresponding to the three mentioned years are: $a=69.0532$, $b=3.45926 \cdot 10^{-7}/3$ and $c=-1.39211 \cdot 10^{-6}/3$.

Let $od((j,k) \rightarrow (j',k'))$ be the *output population diffusion* from cell *(j,k)* to cell *(j',k')*. Taking into account Eq. 2.2, $od((j,k) \rightarrow (j',k')) = id((,j',k') \leftarrow (j,k))$ holds. Thus, the balance diffusion rate of population between districts, $dife((j,k),(j',k'))$ (the dependence on cohorts is not considered here), is:

$$dife((j,k),(j',k')) = 2 \cdot c \cdot \frac{(poba(t,j',k') \cdot poba(t,j,k))}{\sqrt{(j-j')^2 + (k-k')^2}} \quad \text{(Eq. 5.2)}$$

Consequently, *tdif=2·c*. Finally, in order to introduce the dependence on the *i*-th. cohort, Eq. 5.2 is multiplied by the variable CFMI (composition of families per cohorts). Therefore, the final result for the balance diffusion rate of the populationbetween districts per cohorts, DIFE, is:

$$dife\big((i,j,k),(i,j',k')\big) = tdif\,\frac{\big(poba(t,j',k')\cdot poba(t,j,k)\big)\cdot cfmi(t,i)}{\sqrt{(j-j')^2+(k-k')^2}} \qquad \text{(Eq. 5.3)}$$

5.2 Steps to build the Reaction-Diffusion model corresponding to the *city model*

In order to compare the DMDS with another model (for instance the Reaction-Diffusion model), not only theoretically (such comparison has been performed in Section 3.1) but also practically, the *city model*will usethis alternative approach. Thus, the following equation has to be solved:

$$\frac{\partial pobl}{\partial t}(t,\vec{m}) = D\nabla^2 pobl(t,\vec{m}) + \underbrace{crec(t,\vec{m}) - defu(t,\vec{m}) + xmig(t,\vec{m})}_{f(t,\vec{m})}$$

The corresponding steps necessary to reach such target are the following:

Step 1

- Input-variables:

  NUCO: number of cohorts. **NUDX**: number of longitude steps. **NUDY**: number of latitude steps. **TNAC**: birth rate ($^{0}/_{00}$). **D**: Diffusion coefficient, representing the migration rate between districts (cells). **XACO(NUCO-1)**: number of years of each cohort except the last one. **TDEF(NUCO):** death rate. **SMIG**: migratory balance. **DDDT**: Time increment. **DDXY**: Area of each district or cell.

- State-variables:

  POBI(NUCO,NUDX+2,NUDY+2): initial population density per cohorts and districts.**POBL(NUCO,NUDX,NUDY):** population density per cohorts and districts. **PRXI(NUCO,NUDX+1, NUDY):** Initial unitary variation of the population (initial value for P1RX). **PRYI(NUCO, NUDX,NUDY+1):** Initial unitary variation of the population (initial value for P1RY). **P1RX(NUCO,NUDX+1,NUDY+1):** Partial derivative of population respect to X. **P1RY(NUCO,NUDX+1,NUDY+1):** Partial derivative of population respect to Y.

- Auxiliary variables:

  CFMI(NUCO): composition of families per cohorts**. CREC(NUCO,NUDX,NUDY):** births and growing rates per cohorts and districts. **DEFU(NUCO,NUDX,NUDY)**: deaths per cohorts and districts.

POBT: total population at the beginning of each year. **POBF(NUCO)**: total population per cohorts. **XMIG(NUCO,NUDX,NUDY)**: migratory balance per cohorts and districts. **POBA(NUDX,NUDY)**: total population per districts. **DIFE(NUCO,NUDX,NUDY,NUDX,NUDY):** balance diffusion rate of population between districts per cohorts. **P2X2(NUCO,NUDX,NUDY):** Second partial derivative of population respect to X. **P2Y2(NUCO,NUDX,NUDY):** Second partial derivative of population respect to Y.

Steps 2 and 3

Similar to those of DMDS.

Step 4

The equations are the same than DMDS except for POBL, which in this case is:

$$
\begin{cases}
pobl(t,\vec{m}) = \quad pobi(t,\vec{m}) + \dfrac{dddt}{ddxy}(crec(t,i,j,k) - crec(t,i+1,j,k) - defu(t,\vec{m}) + xmig(t,\vec{m}) + \\
\quad + D\cdot(p2x2(i,j,k) + p2y2(i,j,k))); \qquad \text{if } i < \text{nuco} \\
pobl(t,\vec{m}) = pobi(t,\vec{m}) + \dfrac{dddt}{ddxy}(crec(t,i,j,k) - defu(t,\vec{m}) + xmig(t,\vec{m}) + \\
+ D\cdot(p2x2(i,j,k) + p2y2(i,j,k))) \qquad \text{if } i = \text{nuco}
\end{cases}
$$

$$
p1rx(t,\vec{m}) = (pobi(t,i,j+1,k) - pobi(t,i,j,k))/ddxy
$$
$$
p1ry(t,\vec{m}) = (pobi(t,i,j,k+1) - pobi(t,i,j,k))/ddxy
$$

$$
p2x2(t,\vec{m}) = (prxi(t,i,j+1,k) - prxi(t,i,j,k))/ddxy
$$
$$
p2y2(t,\vec{m}) = (pryi(t,i,j+1,k) - pryi(t,i,j,k))/ddxy
$$

$$
prxi(t,\vec{m}) = p1rx(t,\vec{m}) \quad if\ t = dt
$$
$$
pryi(t,\vec{m}) = p1ry(t,\vec{m}) \quad if\ t = dt
$$

Steps 5 and 6

Similar to those of DMDS.

5.3 Simulation and validation

5.3.1 Using the automatic programming tool SIGEM

SIGEM generates programs written in Visual Basic starting from a list of names of variables and a list of equations/tables/rules. Each list is written in a respective text file (.txt). SIGEM and the book byCaselles (2008) are available at http://www.uv.es/caselles.

The *city model simulator*generated by SIGEM has been run with a 425 Mhz. PENTIUM IV processor, with 198 Mb RAM. A simulation with DMDS lasted 4 seconds, and with RD lasted 6 seconds.

5.3.2 Validation of both models DMDS and RD

The common values for DMDS and RD corresponding to the initial conditions are the following:

NUCO = 3. NUDX = 79. NUDY = 10. TNAC = 8.65241421 $^0/_{00}$ .XACO(1) = 14 years. XACO(2) = 50 years. TDEF(1) = 0.548370017 $^0/_{00}$. TDEF(2) = 2.934892979 $^0/_{00}$. TDEF(3) = 46.62292294 $^0/_{00}$. SMIG(1997) = -2665. SMIG(1998) = -4513. SMIG(1999) = -3466. SMIG(2000) = 9717. SMIG(2001) = 9717. DDDT = 1 year. DDXY = 4.594 hectares.

In addition, we need to add variable TDIF = -2·1.39211·10-6/3 in the case of DMDS andvariable D = $10^{-3}/3$ in the case of RD.

The results corresponding to both validation simulations are shown in Figure 1. The urban area considered has been normalised using Cartesian coordinates in the adequate range. Historical data (population densities: inhabitants/4.594 hectares) correspond to the background of each picture using a grey scale represented on the right bar close to each picture. Corresponding simulated data are represented by the "level curves". This is an intuitive or visual form of validation. A possible numerical form of validation is calculating the parameter R^2 (see Section 5 step 5) that appears at the bottom of each figure.

5.3.3 Some instance simulations performed with the *city model*

Taking into account that the city model can be considered as a validated DMDS for demographic predictions, and with the intention of running the sixth step provided in Section 5.1, as an instance, some simulations have been performed. The population density evolution per districts and cohorts to year 2002 has been performed, using as initial values those corresponding to year 2001 in Valencia (see Figure 2). This simulation runsto perform the forecasts corresponding to three different scenarios determined by the input-variable SMIG (the other input-variables conserve the same values than in the validation runs). These three scenarios and the corresponding results are shown as contour plots where longitudes are represented in abscises and latitudes in ordinates:

- **Optimistic Scenario**. Migration in the city is positive. An average of about 9717 persons per year (real migration of the 2001 year) enters the city, during the three years of simulation.
- **Neutral Scenario**. Migration is 0 people per year as an average, during the three years of simulation.
- **Pessimistic Scenario**. Migration is negative. An average of about 9717 people leaves the city per year (the opposite value of the optimistic scenario), during the three years of simulation.

Figure 2 do not show differences inthe population density between scenarios because only one year is forecast, but this is not an objective for this paper. However, these forecasts point out that the optimistic scenario drives the system to equilibrate the proportion of the younger population with respect to the older one, while the neutral and the pessimistic scenarios drive the system to increase this proportion. Take into account that, in these scenarios, the variation of the birth and death rates has not been considered. Thus, it is understood that considering more complex and realistic scenarios, and due to the city model can be considered as a validated model, forecasts about the evolution of the population density per cohorts could be considered as acceptable under the respective scenarios. Therefore, possible policies about school and health needs and other services, distributed per districts, could be based on the forecast evolution of the population density under such scenarios.

6. Final remarks

The main goal of this paper has been to suggest a formalism based on an equation, the DMDS, in order to embed existing dynamic models including space-time variation of systems, and to adapt the methodology proposed by Caselles (1994) to build models of DMDS type. The DMDS suggested in (Eq.2.4) has been derived by three different methods:

1. By introducing space in classical models of systems with time dynamics, deriving an equation, called STMS (Micó and Caselles, 1998), which is a first approach to the DMDS.
2. By ageneralisationof the reaction-diffusion model, once converted into a finite difference equation.
3. By changing conveniently the way to write the equation of cellular automata models.

An aim of this paper has been to show how these three approaches are particular cases of the DMDS.

Finally, the adaptation of the methodology suggested by Caselles (1994) to the DMDS approach has been used to forecast the evolution of the population density of an urban system by cohorts and districts. This application case is an example of how to adapt the DMDS formalism to a particular case, the city of Valencia (Spain).

A line for future research could be obtaining a validated DMDS of a general urban system where the present model is the corresponding to the demographic subsystem, in the context of the formalism of systems decomposition and coupling stated by Caselles (1993). Thus, this demographic model is the first step towards a general space-time model of an urban system. Other subsystems, such as the corresponding to economy, housing, pollution, structures etc., must be built and validated separately and, later, coupled to form a unique system. Obviously, these subsystems will have to include other state-variables - besides population - referred to space-time distribution of firms, structures, land-use, and so on.

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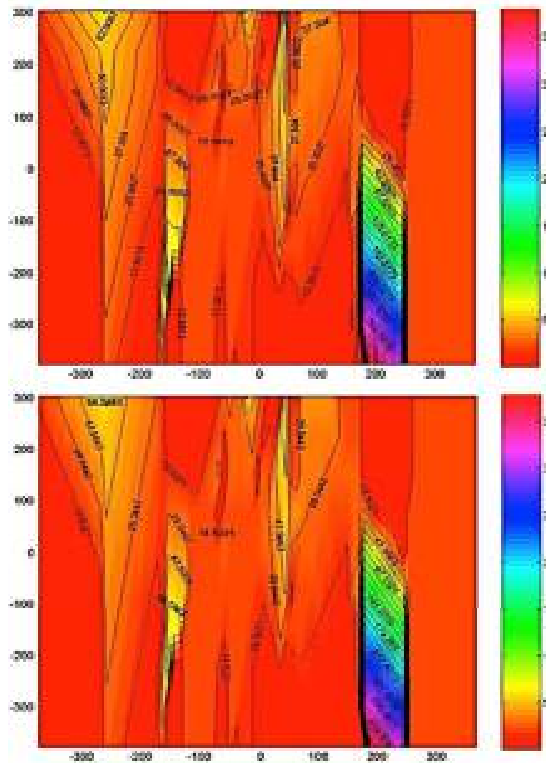
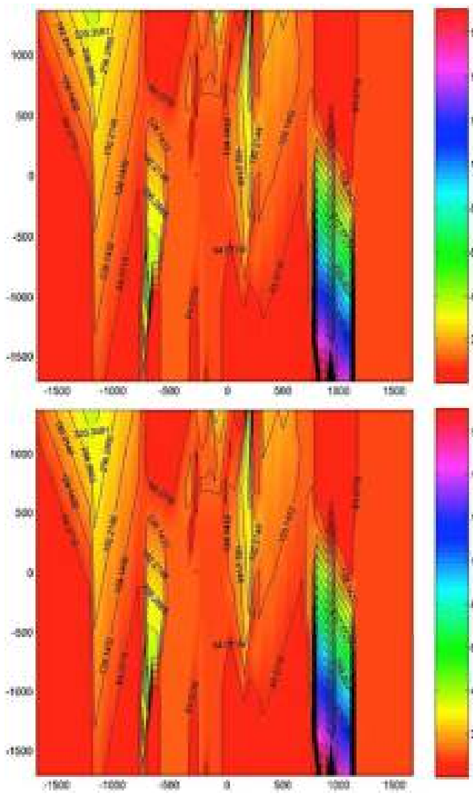
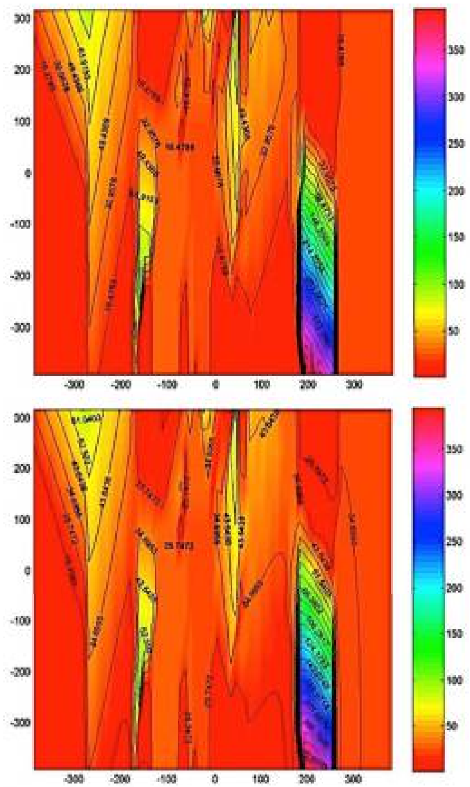
YEAR 1996.



Cohort 1. Up RD (R^2=0.938). Low DMDS (R^2=0.985).

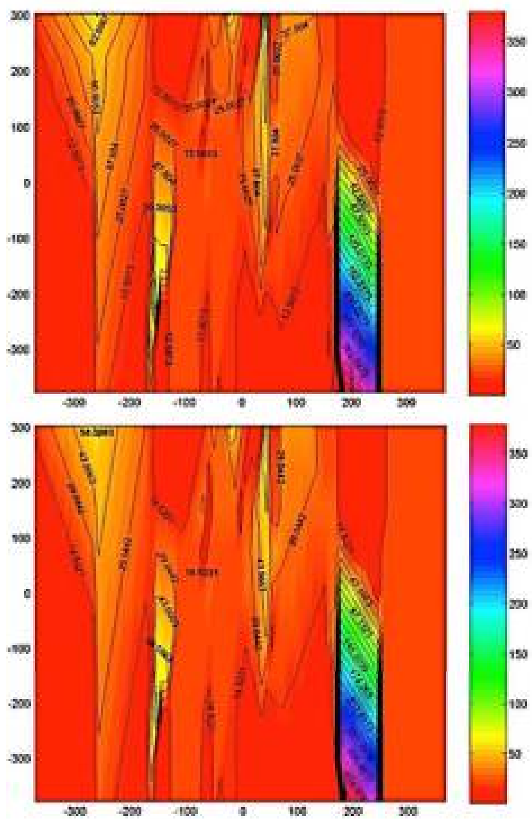


Cohort 2. Up RD (R2=0.985). Low (R2=0.988).

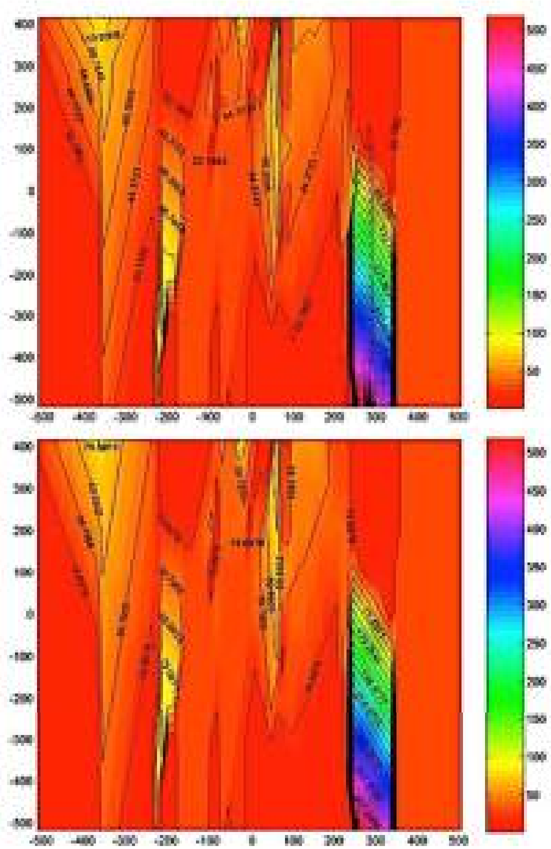


Cohort 3. Up RD (R^2=0.931). Low DMDS (R^2=0.958).

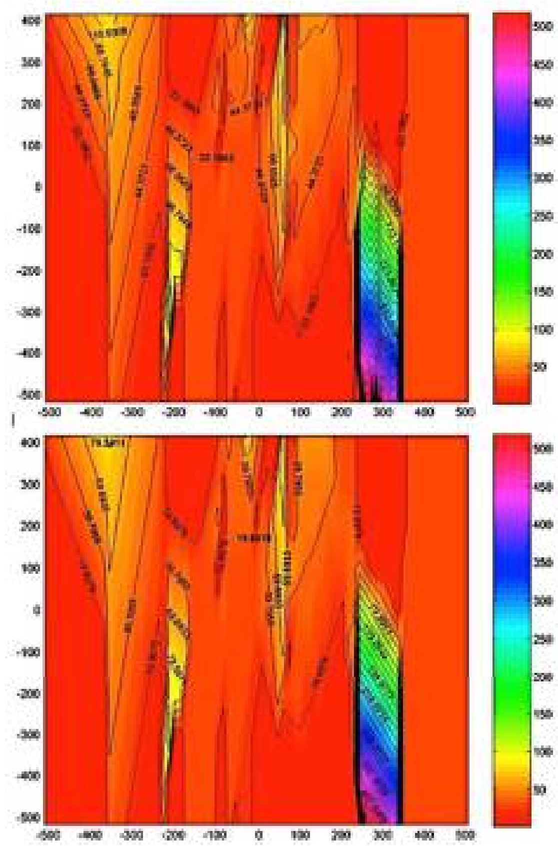
YEAR 2001



Cohort 1. Up RD (R^2=0.8921). Low DMDS (R^2=0.9107).



Cohort 2. Up RD (R2=0.8852). Low (R2=0.9321).



Cohort 3. Up RD (R^2=0.9039). Low DMDS (R^2=0.9616).

Figure 1. Validation of the DMDS model by cohorts.

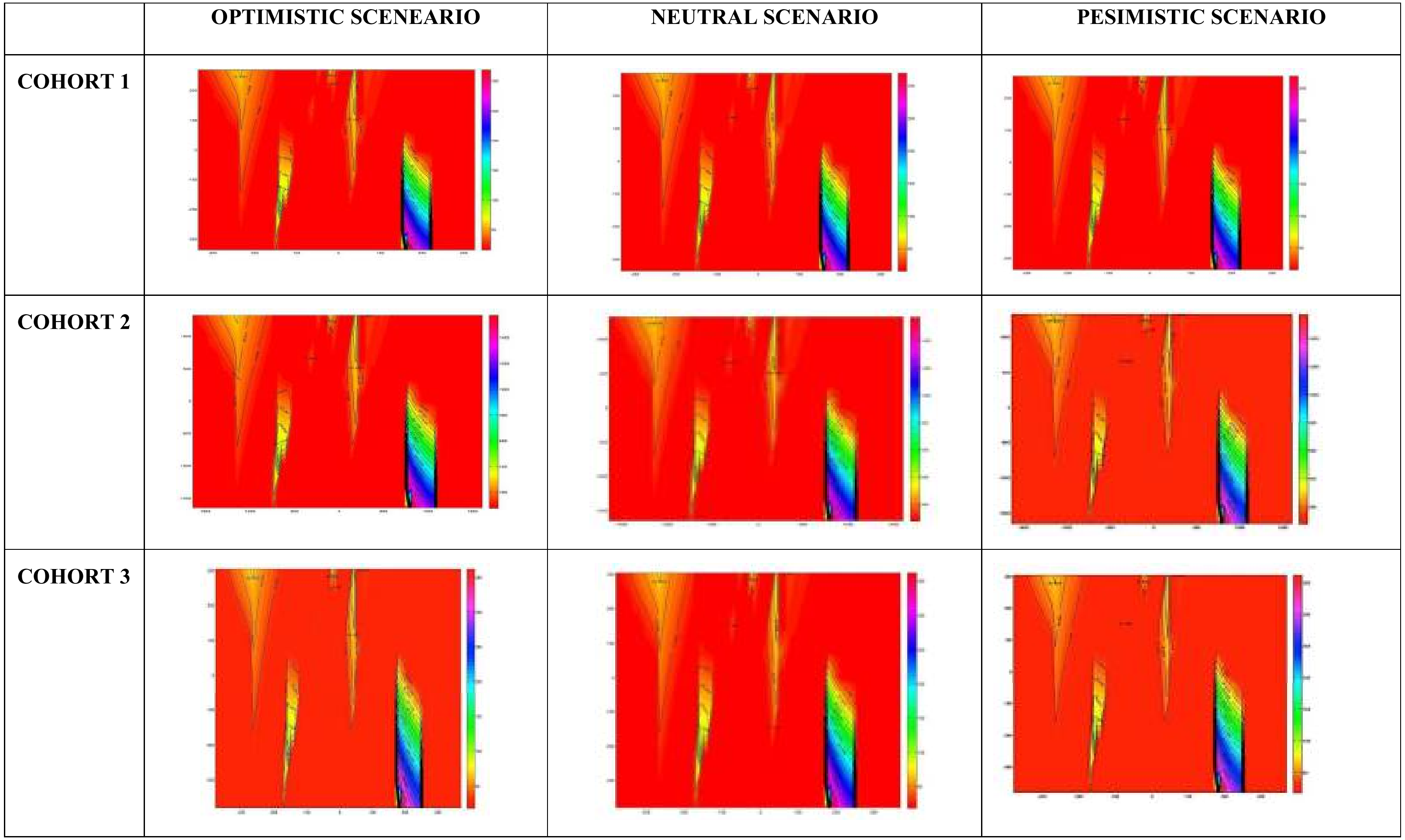


Figure 2. From up to down, population density for cohort 1 (0-14 years), cohort 2 (15-64 years) and cohort 3 (more than 64 years), for Valencia city given by the city model for 2002.