Differential Equations and Carathéodory Solutions: How System Dynamics Describes Formal Dynamical Systems

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Abstract. It is often informally stated that system dynamics (SD) models are equivalent to differential equation systems. This paper formalizes the concept of an SD model as a collection of rate equations, auxiliary equations, and the "flow coupling" of flows to stocks. If such a model has no causal loops that consist only of auxiliaries, then it is possible to find an equivalent differential equation system. The generalized solution concept of Carathéodory is shown to be suitable for defining the corresponding state transition map, which leads to a formal dynamical system.

Introduction

According to Hinrichsen and Pritchard [1], a dynamical system is a structure that consists of a time set (i.e., a totally ordered set of all time values) $\mathbb{T}$, an input value set U, an input function space $\mathscr{U} \subset U^{\mathbb{T}}$, a state space X, an output space Y, and two maps: the state transition map ϕ and the output map η. For every initial value $x_0 \in X$ at time point $t_0 \in \mathbb{T}$, every input signal $u \in \mathscr{U}$ and every time point $t \in \mathbb{T}$ such that $(t;t_0,x_0,u) \in D_\phi \subset \mathbb{T}^2 \times X \times \mathscr{U}$, ϕ maps to the state $x = \phi(t;t_0,x_0,u) \in X$. The output map then produces the corresponding output value $y = \eta(t,x,u(t)) \in Y$.

Four axioms must hold for the state transition map:
Interval Axiom: For every fixed initial value x_0, initial time t_0, and input signal u, ϕ is defined on an interval in $\mathbb{T}$ that contains t_0.
Consistency Axiom: For $t = t_0$, ϕ always maps to the initial value x_0.
Causality Axiom: If two input signals u and v equal each other on the interval between t_0 and t_1, then $\phi(t_1;t_0,x_0,u) = \phi(t_1;t_0,x_0,v)$.
Cocycle Property: If we "restart" the system at time $t_1 > t_0$, we get the same state at time $t_2 > t_1$ as if we go directly to t_2 from t_0, because $\phi(t_2;t_0,x_0,u) = \phi(t_2;t_1,\phi(t_1;t_0,x_0,u),u)$.

It is often informally stated that every system dynamics (SD) model is equivalent to a system of differential equations and thus a dynamical system. Basically, every stock or level stands for one differential equation, which describes the change of the stock over time. In this paper, we show formally that this is indeed true.

Note. This article is a revised version of Section 3.4 of the author's PhD thesis [2].

1 The Building Blocks of System Dynamics Models

1.1 Stocks and flows

One major advantage of SD is that only a few basic elements are necessary to build a model. Every SD model consists of *stocks* and *flows* (equivalently, they are often called *levels* and *rates*). Stocks are variables that accumulate a certain quantity. Through this accumulation, stocks represent the memory and state of the system.

Flows are the other important variable type. They have no memory, because at every time point, their value depends only on the current values of the stocks. But they represent stock changes, because flows are the sole quantities that the stocks directly accumulate. More specifically, a flow F may be an inflow of a certain stock S, in which case S is increased by F, or it may be an outflow of S, in which case S is decreased by F.

These two elements are enough to describe the entire dynamics of a system. Actually, as we will show, if the dependence of the flows on the stocks is specified through equations, the system is equivalent to a system of ordinary differential equations, where the stocks are the state variables and the flows are the right-hand sides of the differential equations. Together with initial values for the stocks, an initial value problem is given, which has a unique solution under the condition well-known from the theory of differential equations that the right-hand side is continuous in time and Lipschitz continuous in the state variable. In this regard, SD is just another way of describing differential equations.

However, the systematic way of deriving the equations is the real benefit of the method. The stock and flow structure is important on its own, even without the equations, because even it alone gives qualitative insight into the possible and probable dynamic behaviour of a system. Moreover, it has a standardized graphical notation, the *stock and flow diagram*. Figure 1 shows a simple stock and flow diagram.

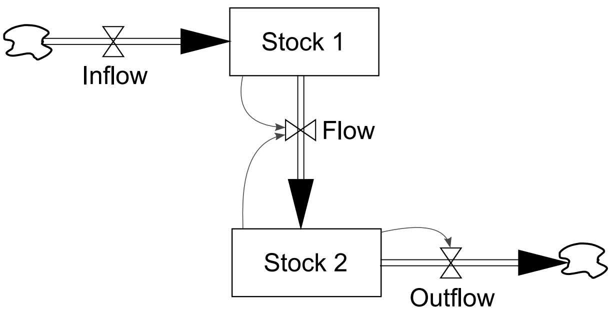

Figure 1: A stock and flow diagram that consists only of stocks (depicted as boxes) and flows (depicted as pipes with valves in the middle). If the source or sink of a flow is not important because it lies outside the system boundary, a small cloud symbol is drawn instead. Blue arrows show causal dependencies.

In the diagram, boxes depict stocks and pipes with valves in their middle depict flows. Every flow that ends in a stock is an inflow for this stock, whereas every flow that begins in a stock is an outflow. Stock 1 has one inflow that begins in a source outside the model boundary, depicted by a cloud symbol. Similarly, an outflow goes from Stock 2 into a sink. The flow in the middle is both an outflow for Stock 1 and an inflow for Stock 2.

There is an additional causal structure in the diagram. The blue arrows show on which stocks the flows depend. For example, the flow between Stock 1 and Stock 2 depends on both of them. On the other hand, it would be an error to use Stock 1 in the equation of the outflow from Stock 2, because there is no blue arrow from Stock 1 to Flow, which means that it is independent of Stock 1. Fortunately, SD simulation software is capable of automatically detecting such inconsistencies between diagram and equations.

1.2 Auxiliaries and constants

Stock and flow diagrams with only stocks, flows, and their causal dependencies along with equations could describe every possible SD model, but often different concepts and effects are involved in a flow equation. In this case, it is beneficial to include intermediary variables to state these relationships directly in the stock and flow diagram. They are called *auxiliaries* because of their not necessary but often helpful nature. Like flows, these variables can depend on stocks and other auxiliaries. It must always be possible to calculate their value from all values of the stocks.

Additionally, stock and flow diagrams can include constant values as separate quantities. Of course, it would be possible to just write these values in the equations of auxiliaries or flows, but as in computer programming the use of such "magic numbers" is considered to be bad practice. The SD methodology tries to encourage modellers to make concepts graphically explicit and to give them meaningful names.

2 Formal Definition of SD Models

Definition 2.1 (System Dynamics Model)**.** A *system dynamics model* with m stocks (levels), n flows (rates), k_a auxiliaries, and k_p parameters consists of n flow or rate equations $f_i\colon D_{f_i} \to \mathbb{R}$, $i \in \{1,\dots,n\}$, where $D_{f_i} \subset \mathbb{R}^m \times \mathbb{R}^{k_a} \times \mathbb{R}^{k_p}$, k_a auxiliary equations $g_j\colon D_{g_j} \to \mathbb{R}$, $j \in \{1,\dots,k_a\}$, where $D_{g_j} \subset \mathbb{R}^m \times \mathbb{R}^{k_a} \times \mathbb{R}^{k_p}$, and the flow coupling $FC \in \left(\{0,\dots,m\}^2 \setminus \{(i,i) : i \in \{0,\dots,m\}\}\right)^n$.

The flow coupling FC denotes which stocks a flow connects. Here, the index 0 represents a source or sink. The pair $(i,0)$ in the flow coupling stands, for example, for a flow from the i-th stock into a sink. A flow from the i-th stock into the stock with index j would be represented by the pair (i,j).

All variables of a system dynamics model have values in $\mathbb{R}$. We write $\mathbf{x}(t) \in \mathbb{R}^m$ for the state vector of stocks at time t, $\mathbf{r}(t) \in \mathbb{R}^n$ for the vector of flows, $\mathbf{a}(t) \in \mathbb{R}^{k_a}$ for the vector of auxiliaries, and $\mathbf{p} \in \mathbb{R}^{k_p}$ for the parameter vector.

3 Causal Loops

In the following, we want to find a corresponding differential or integral equation system for an SD model and define the state transition mapping and the output mapping via the solution of this equation system. This is impossible if the equations for the auxiliary variables form *algebraic loops*: Suppose that there are three auxiliary variables a_1, a_2, and a_3 in the model, and that the equations are $a_1 = g_1(\mathbf{x},\mathbf{a},\mathbf{p}) = a_2$, $a_2 = g_2(\mathbf{x},\mathbf{a},\mathbf{p}) = a_3$, and $a_3 = g_3(\mathbf{x},\mathbf{a},\mathbf{p}) = a_1$. Obviously, the equations are redundant and reduce to $a_1 = a_2 = a_3$, which has infinitely many possible solutions.

The question is which preconditions secure that there are no algebraic loops involving auxiliaries. This involves the concept of causal links.

Definition 3.1 (Causal Link)**.** In a system dynamics model, a variable v_1, where v_1 is a stock, an auxiliary, or a parameter, is a *direct cause* of an auxiliary or flow v_2 if the corresponding auxiliary equation g_j (or f_j) depends on v_1, that is, if the value of g_j (or f_j) is not the same for all values of v_1, where all other variables are fixed. Likewise, a flow v_1 is a direct cause of a stock v_2 if it is an outflow or inflow of v_2. In both cases, the model has a *causal link* from v_1 to v_2.

Beginning from a variable, it is possible to follow causal links.

Definition 3.2 (Causal Chain)**.** A sequence $v_1,\dots,v_k$ of variables with $k \in \mathbb{N}$ is called a *finite causal chain* of length k beginning at v_1 if for every $i \in \mathbb{N}$ with $1 \le i < k$ there is a causal link from v_i to v_{i+1}. Likewise, a sequence $(v_i)_{i\in\mathbb{N}}$ is called an *infinite causal chain* beginning at v_1 if it has the same property as in the finite case.

Definition 3.3 (Causal Loop)**.** A *causal loop* of length k is a finite causal chain $v_1,\dots,v_k$ where $v_1 = v_k$ and $v_i \neq v_j$ if $1 < i < k$ or $1 < j < k$.

If and only if there is a causal loop that involves just auxiliary variables the equations form an algebraic loop.

4 The Link Matrix

We will now define a matrix that stores all causal links between auxiliaries. It is possible to see if an SD model includes a causal loop with only auxiliary variables from the structure of this matrix.

Definition 4.1 (Link Matrix)**.** The *link matrix* L of an SD model with auxiliary variables $a_1,\dots,a_{k_a}$ is the matrix where $L_{i,j}$ is 1 if there is a causal link from a_i to a_j and 0 otherwise.

Obviously, auxiliaries that have only causal links to flows do not pose any problem. But also other auxiliaries with causal links only to these first kind of auxiliaries cannot be part of an algebraic loop. We can pursue this strategy further and thus classify them:

Definition 4.2 (Causal Order)**.** An auxiliary is of *causal order* 0 if it has no causal link to any other auxiliary. It is of order 1 if it has only causal links to auxiliaries of order 0. Generally, an auxiliary has causal order n if it has links to auxiliaries of order $n-1$, but not causal links to auxiliaries of higher order. All other auxiliaries have infinite causal order.

Lemma 4.3. *An auxiliary a_0 has infinite causal order if and only if it is part of a causal loop involving only auxiliaries or if there is a causal chain beginning at a_0 that ends in such a causal loop.*

Proof. No auxiliary in a causal loop has causal order 0, because every auxiliary in the loop has a causal link to the next auxiliary in the loop. It follows that also no auxiliary can be of order 1, because an auxiliary of order 1 only has links to order-0 auxiliaries. The same holds for every finite order. Finally, if a causal chain ends in an auxiliary that is part of a causal loop, all auxiliaries of the causal chain have infinite order, which can be seen recursively.

On the other hand, suppose that a_0 is not part of a causal loop with only auxiliaries and there is also no causal chain beginning at a_0 that ends in a loop. As there are only k_a auxiliaries and no auxiliary can be part of a causal chain twice if the chain contains no loop, every causal chain that starts at a_0 is finite. If a_0 has infinite order, at least one of the auxiliaries to whom it has a causal link, denoted by a_0', has to have infinite order too. Again, one of the auxiliaries to whom a_0' has a causal link has to have infinite order. In this way, it would be possible to construct an infinite causal chain where every auxiliary has infinite order, which is in contradiction of the fact that every causal chain starting from a_0 is finite. □

Figure 2 shows an example of a causal diagram with only auxiliary variables. All auxiliaries in the loop have infinite causal order. Additionally, a_0 has infinite causal order because it has a link to another auxiliary of infinite order. The other auxiliaries (a_5, a_6, and a_7) have finite order.

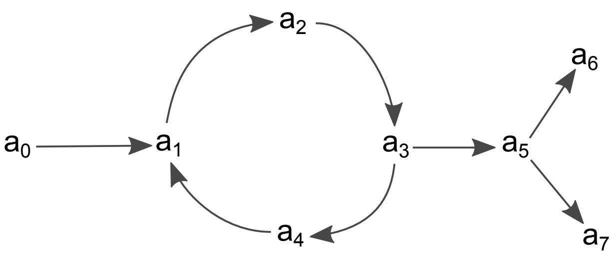

Figure 2: In this causal diagram, a_6 and a_7 have causal order 0 (they have no link to any other auxiliary). The only other variable with finite causal order is a_5, which has causal order 1 because it has only links to variables of order 0. All other auxiliaries in the diagram have infinite causal order.

Proposition 4.4. *An SD model contains a causal loop involving only auxiliaries if and only if it is not possible to renumber the auxiliaries such that the link matrix is a lower triangle matrix.*

Proof. First, suppose that the model has a causal loop involving only auxiliaries. For the link matrix to be a lower triangle matrix, a variable a_i can only have a causal link to a_j if $j < i$. One variable a' of the causal loop has to be the variable with the lowest number of all variables in the loop. As a variable in the loop, it has a causal link to the next variable in the loop. This variable must then have a lower number then a', which leads to a contradiction. Therefore, the link matrix cannot be of lower triangular form.

Now suppose that no causal loop involves only auxiliaries. Lemma 4.3 shows that then all auxiliaries must have finite causal order. We can therefore numerate the auxiliaries according to their order: First, we take all order-0 auxiliaries, then all order-1 auxiliaries, and so on. Each auxiliary can have only links to auxiliaries with lower order, which shows that the link matrix is of lower triangular form. □

5 Flow Equations of a System Dynamics Model

The last proposition gives a characterisation of the system dynamics models whose equations do not form algebraic loops. These models allow for the formation of a differential equation system which depends only on the values of stocks and parameters.

Proposition 5.1. *If a system dynamics model contains no causal loops of only auxiliaries, the flow equations can be written just in terms of stocks and parameters.*

Proof. In a system dynamics model, the flow equations might be given as functions that depend not only on stocks and parameters, but also on the values of auxiliaries. However, according to Proposition 4.4, the auxiliaries of a system dynamics model without algebraic loops can be enumerated such that the link matrix is of lower triangular form. The value of the first auxiliary a_1 depends only on stocks and parameters, that is, there is a function $g'_1 : D'_{g_1} \to \mathbb{R}$ such that $g'_1(\mathbf{x}(t), \mathbf{p}) = g_1(\mathbf{x}(t), \mathbf{a}(t), \mathbf{p})$ for all $(\mathbf{x}(t), \mathbf{a}(t), \mathbf{p}) \in D_{g_1}$, where the domain D'_{g_1} is the restriction of D_{g_1} to the set $\mathbb{R}^m \times \mathbb{R}^{k_p}$. The second auxiliary a_2 may depend on a_1 as well, but as the value of a_1 is a function of only stocks and parameters, so is a_2. In general, as a_i for $1 \leq i < k_a$ depends only on stocks and parameters, so does a_{i+1} .

Finally, as all auxiliaries can be written as functions of stocks and parameters, all flow equations are also only functions of stocks and parameters. □

6 The State Transition Map of a System Dynamics Model

The result from the last section guarantees that it is possible to find a differential equation system that is equivalent to the system dynamics model. Two problems could arise:

1. The differential equation system might not have a solution.
2. The differential equation might have more than one solution.

In both cases, it is not clear how to define the state transition mapping of the corresponding dynamical system. We should thus require the differential equation system to have a unique solution.

Is it enough if we allow for solutions in the classical sense? Consider, for example, the first order system

$$\begin{aligned} \frac{dy}{dt} &= u - y \\ y(0) &= 0 \end{aligned} \tag{1}$$

where u is the input function and y is the output function. If u is continuous, then the right-hand side of Equation 1 is continuous and therefore the initial value problem has a solution according to the Peano existence theorem. (It is even unique because the right-hand side is Lipschitz continuous in y.) But if u is not continuous, a solution might not exist, such as in the case where the input u is the Heaviside step function

$$\begin{aligned} H\colon \mathbb{R} &\to \{0,1\} \\ t \mapsto H(t) &:= \begin{cases} 1 & \text{for } t \geq 0 \\ 0 & \text{for } t < 0. \end{cases} \end{aligned}$$

Proposition 6.1. *The initial value problem* (1) *with input $u = H$, where H is the Heaviside step function, has no solution in the classical sense.*

Proof. A solution y would have to fulfill

$$\frac{dy}{dt}(t) = \begin{cases} -y(t) & \text{for } t < 0 \\ 1 & \text{for } t = 0, \end{cases}$$

and as a differentiable function it must be continuous. Since $y(0) = 0$, for $\varepsilon > 0$ there exists a $\delta > 0$ such that $|y(t)| < \varepsilon$ for all t with $|t| < \delta$. In particular, for $\delta < t < 0$ we have $|\frac{dy}{dt}(t)| = |-y(t)| < \varepsilon$. If we choose, for example, $\varepsilon = \frac{1}{2}$, we can therefore fix a point $t_1 < 0$ such that $y(t) < \frac{1}{2}$ for all t with $t_1 \leq t < 0$. But as a derivative, $\frac{dy}{dt}$ must have the intermediate value property according to Darboux's theorem and, therefore, take all values between $\frac{dy}{dt}(t_1)$ and $\frac{dy}{dt}(0) = 1$ on the interval $[t_1, 0]$, which leads to a contradiction. □

This is unsatisfactory, as the Euler method that is typically used for the simulation of SD models does not have any problems with this system. Only the first step, which can be made arbitrarily small, is affected by the discontinuity. For all further steps, the input function equals 1.

It is possible to solve the differential equation for $t \geq 0$ with variation of constants and ignore the discontinuity at $t = 0$, which leads to the solution $y(t) = 1 - e^{-t}$. For $t < 0$, we can set $y(t) = 0$. The "solution" has the following properties:

1. It is Lipschitz continuous.
2. It fulfils the differential equation for $t \neq 0$.

It seems natural to accept this function as a solution. This leads to one kind of a generalized or weak solution concept: a solution in the sense of Carathéodory.

Definition 6.2 (Carathéodory Solution)**.** A function is a *Carathéodory solution* of an ordinary differential equation system on an interval $I \subset \mathbb{R}$ if it is absolutely continuous and satisfies the differential equations almost everywhere on I.

The function y in the example above is absolutely continuous, because it is even Lipschitz continuous, and it satisfies the differential equation everywhere apart from $t = 0$, that is, almost everywhere, thus it is a Carathéodory solution. Note that an absolutely continuous function is differentiable almost everywhere. For comparisons with other generalized solution concepts, see [3].

Definition 6.3 (State Trajectory of a System Dynamics Model)**.** Let $\mathscr{M}_{SD}$ be a system dynamics model with no algebraic loop. The differential equation system

$$\frac{d\mathbf{x}}{dt}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{p}), \tag{2}$$

where $\mathbf{x}(t)$ is the state vector containing the values of the stocks, $\mathbf{p}$ is the parameter vector, and $\mathbf{f}$ is the vector of flow equations that depends only on the stocks and the parameters as in Proposition 5.1, is called the *equivalent differential equations system* of $\mathscr{M}_{SD}$. For an initial state x_0 at time t_0, a Carathéodory solution of this system is called a *state trajectory* of the system dynamics model.

Through this definition, it is possible to specify a state transition map that corresponds to the SD model. For every fixed values of t_0 and x_0, we can set it to the value of the state trajectory on the maximum interval where a unique Carathéodory solution exists. It is permissible that this interval contains only t_0. Obviously, the state transition map obeys the other necessary properties such as consistency. Note that a system dynamics model has no separate input variables. Therefore, the input space of the corresponding dynamical system consists only of one element.

There is no single correct choice for an output map. An SD model usually has no dedicated output variables.

However, the values of all stocks and auxiliaries can be seen as output. The output space is then $\mathbb{R}^m \times \mathbb{R}^{k_a}$.

7 Conclusions

Systems theory can serve as a rigorous mathematical foundation for modelling and simulation. In this paper, we have shown that system dynamics is indeed a method that specifies dynamical systems. While differential equations are not specified directly, each feasible SD model has an equivalent differential equation system.

We can see an SD model as a collection of stocks, flows, auxiliaries, and parameters together with rate equations and auxiliary equations. Additionally, it must be specified which stocks are coupled by flows (flow coupling).

SD models are not allowed to have algebraic loops, where only auxiliary variables depend on each other without any accumulating stock in between. We have proposed formal definitions of causal links, causal chains, and causal loops, which make it possible to show that if there are no algebraic loops, (i.e., no causal loops of only auxiliaries) the flow equations of the SD model can be written just in terms of stocks and parameters. Thus, the model has an equivalent formulation as a differential equation system.

Moreover, the links between auxiliaries form a link matrix, and the model has no algebraic loops if and only if it is not possible to transform this matrix into a lower triangle form by renumbering the auxiliaries.

These findings can serve as a basis for a formal system theoretical treatment of SD models. They also show that a generalized solution concept such as the one of Carathéodory is necessary, because in applications of SD the right-hand sides can have discontinuities.

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