# Description of continuum state cellular automata using ordinary differential equations

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## 1 – Notations (see also [Van et al 04])

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|---|---|
| $\Gamma$ | Cellular space (the set of all the cell subdividing the urban space). |
| $E_c = \mathbb{R}^d$ | Configuration space of the cell $c \in \Gamma$. |
| $E = \oplus_{c \in \Gamma} E_c$ | Configuration space of the system |
| $A$ | Set of all elementary processes. |
| $V_\alpha = R^{n(\alpha)}$ | Vector space of the goods produced in an elementary event $\alpha \in A$. |
| $D = \Gamma \times A \times V_\alpha$ | Decision space. A point in $D$ represents a $(c, \alpha, \pi)$-event, that is an event of the kind $\alpha \in A$ taking place in the cell $c \in \Gamma$ with continuum parameters $\pi \in V_\alpha$. |
| $\lambda_{c,\alpha} : E \times V_\alpha \to \mathbb{R}_+$ | Density of intensity for events. $\lambda_{c,\alpha}(e, \pi)$ is the density of intensity of an $(c, \alpha, \pi)$-event. |
| $\gamma_{c,\alpha}$ | Set of functions describing the transformation of the state vector of the system when a $(c, \alpha, \pi)$-event occurs. |

The functions $\gamma_{c,\alpha}$ defined above acts in the following way (see equation 3.3.3. in [Van et al 04]):

$$\gamma_{c,\alpha} : E \times V_\alpha \to E$$
$$(e,\pi) \mapsto \gamma_{c,\alpha}(e,\pi) = e + \sum_{j=1}^{n(\alpha)} \pi_j \eta_{c,\alpha}^j \qquad (1.1)$$

where $\pi = \left(\pi_1, \pi_2, \ldots, \pi_{n(\alpha)}\right) \in V_\alpha$ and $\eta_{c,\alpha}^j$ are vectors. The transformation rule (1.1) is linear because we have chosen to describe the configuration of the system by means of extensive quantity like volumes and surfaces (they increment additively).

## 2 – The time evolution of the Cellular Automaton as a Markov jump process.

The assumption (see the preprint of the paper in this web page) that all the elementary processes are Poisson distributed during a short time interval $\Delta t$ leads naturally to a description of the CA through a Markov jump process (MJP). In such kind of continuum time stochastic processes the system passes through a sequence $e_1, e_2, e_3 \cdots$ of states jumping from the state $e_n$ to the state $e_{n+1}$ at the stochastic time $t_n$. The difference $\theta = t_{n+1} - t_n$ is the sojourn time on the state $e_n$.

Markov jump processes are characterized by exponentially distributed sojourn time on a state are:

$$P\{\theta \le t\} = \exp\left(-\lambda(e) \cdot t\right) \qquad (2.1)$$

where $\lambda$ is the intensity of the process depending in general upon the state $e$.

It is possible to show that, if the sojourn times on a state are exponentially distributed, the number of jumps during a small time interval $\Delta t$ is approximately given by a Poisson distribution:

$$P\{N = n\} \cong \frac{1}{n!} \cdot \exp\left(-\lambda \cdot \Delta t\right) \cdot \left(\lambda \cdot \Delta t\right)^n \qquad (2.2)$$

This suggest us using a Markov jump process in order to describe the time evolution of the CA in the limit of a small tile step $\Delta t$. In order to show how this task can be accomplished let us introduce some general topics about MJP.

A MJP is completely specified giving its semimarkov kernel $Q : E \times \mathfrak{B}(E) \times R_+ \to R_+$ where $E$ is the configuration space of the system and $\mathfrak{B}(E)$ are the Borel set of $E$. The function $Q$ must fulfil the following three conditions:

1) for given $B \in \mathfrak{B}(E)$ and $t \in R_+$ the function $Q(\bullet, B, t)$ is measurable;
2) for given $e \in E$ and $t \in R_+$ the function $Q(e, \bullet, t)$ is a measure on $\mathfrak{B}(E)$ such that $Q(e, E, t) \leq 1$ and $Q(e, E, +\infty) = 1$
3) for given $e \in E$ and $B \in \mathfrak{B}(E)$ the function $Q(e, B, \bullet)$ is a probability distribution on $R_+$.

The function $Q(e, B, t)$ must to be interpreted as the probability that the system jumps from the state $e \in E$ into the Borel set $B \in \mathfrak{B}(E)$ with a sojourn time in the state $e$ less that $t$.

In the next section we will construct a semimarkov kernel for a Markov jump process associated to our CA model.

## 2.1 – Semimarkov kernel for the CA

The functions (1.1) define a set of $n(\alpha)$-dimensional affine subspaces $U_{e,\alpha,c}$ in the configuration space $E$ parameterized by $\pi = (\pi_1, \pi_2, \ldots, \pi_{n(\alpha)}) \in V_\alpha$. A point $e' \in U_{e,\alpha,c}$ parameterized by $\pi = (\pi_1, \pi_2, \ldots, \pi_{n(\alpha)}) \in V_\alpha$ represents the configuration reached by the system after a $(c, \alpha, \pi)$-event starting from $e \in E$.

In order to define a semimarkov kernel for a jump process we start defining a set of measure $\delta_{e,\alpha,c}$ concentred on $U_{e,\alpha,c}$ and with density given by the non negative measurable functions $\lambda_{\alpha,c} : E \times V_\alpha \to \mathbb{R}_+$ that define the density of the intensities in the cellular automaton. The measure $\delta_{e,\alpha,c}$ are defined by the following relations:

$$\delta_{e,\alpha,c}(B) = \int_{(\gamma_{\alpha,c})^{-1}(e,B)} \lambda_{\alpha,c}(e, \pi)\, d\pi \qquad (2.1.1)$$

where $B$ is a Borel set in $E$ and with $(\gamma_{c,\alpha})^{-1}(e, B) \in V_\alpha$ we have indicated the counter image of $B$ under the application of $\gamma_{c,\alpha}$ for fixed $e \in E$.

Let us define the total intensity $\Lambda$ of the process in the following way:

$$\Lambda: \quad E \to R_+$$
$$e \mapsto \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V^\alpha}\lambda_{c,\alpha}(e,\pi)\,d\pi \tag{2.1.2}$$

Now we can define a semi Markov kernel in the following way:

$$Q: \quad E\times\mathfrak{B}(E)\times R_+ \to R_+$$
$$Q(e,B,t) = \left(1-\exp(-\Lambda(e)\cdot t)\right)\frac{1}{\Lambda(e)}\sum_{c\in\Gamma}\sum_{\alpha\in A}\delta_{e,\alpha,c}(B) = \tag{2.1.3}$$
$$= \left(1-\exp(-\Lambda(e)\cdot t)\right)\frac{1}{\Lambda(e)}\sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{(\gamma_{\alpha,c})^{-1}(e,B)}\lambda_{\alpha,c}(e,\pi)\,d\pi$$

In order to get an useful interpretation of the kernel (2.1.3) we will evaluate the distribution $\Theta_e$ for the sojourn time on a state $e\in E$ and the transition function of the imbedded Markov chain defined, roughly speaking, as the Markov chain obtained considering only the sequence of the states with no reference to the sojourn times.

The distribution of the sojourn time is obtained substituting $B = E$ in the (2.1.3):

$$\Theta_e(t) := Q(e,E,t) =$$
$$= \left(1-\exp(-\Lambda(e)\cdot t)\right)\frac{1}{\Lambda(e)}\sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha}\lambda_{\alpha,c}(e,\pi)\,d\pi = \tag{2.1.4}$$
$$= \left(1-\exp(-\Lambda(e)\cdot t)\right)$$

where in the last passage we have used the definition (2.1.2) for the total intensity of the process and the trivial relation $\left(\gamma_{c,\alpha}\right)^{-1}(e,E) = V_\alpha$. The (2.1.4) shows that the sojourn time on a the state $e\in E$ is exponentially distributed with intensity $\Lambda(e)$.

The transition function of the embedded Markov chain is defined through the following relation: $Q_0(e,B) := \lim_{t\to+\infty} Q_0(e,B,t)$. The transition function $Q_0(e,B)$ represents hence the probability to have a jump from the state $e\in E$ into the Borel set $B\in\mathfrak{B}(E)$.
We obtain for the kernel (2.1.3):

$$Q_0(e,B) = \lim_{t\to+\infty} Q(e,B,t) =$$
$$= \frac{1}{\Lambda(e)} \sum_{c\in\Gamma} \sum_{\alpha\in A} \int_{(\gamma_{\alpha,c})^{-1}(e,B)} \lambda_{\alpha,c}(e,\pi)\, d\pi := \sum_{c\in\Gamma} \sum_{\alpha\in A} Q_0^{\alpha,c}(e,B) \tag{2.1.5}$$

Intuitively speaking the expression $Q_0^{\alpha,c}(e,B)$ in (2.1.5) represents the probabilities to have a jump of kind $\alpha$ in the cell $c$ from the state $e$ into the Borel set $B$:

$$P\{\pi\in B\subseteq V_\alpha, J=(\alpha,c)\} := Q_0^{\alpha,c}(e,B) =$$
$$= \frac{1}{\Lambda(e)} \int_{(\gamma_{\alpha,c})^{-1}(e,B)} \lambda_{\alpha,c}(e,\pi)\, d\pi \tag{2.1.6}$$

where we have introduced the discrete stochastic variable $J$ that gives the typology $(\alpha,c)$ of the last jump (more precisely it should depends on the time $t$). The equation (2.1.6) is in accordance with the interpretation given in the preprint of the paper of the functions $\lambda_{\alpha,c}$ as density of intensities for the processes.

In the same way we can intuitively construct the conditional probability to have a jump with continuum parameters in a subset $C\subset V_\alpha$ given that the jump is of the kind $\alpha$ and occurs in the cell $c$:

$$P\{\pi\in C\subseteq V_\alpha / J=(\alpha,c)\} = \frac{P\{\pi\in A\subseteq V_\alpha, J=(\alpha,c)\}}{P\{J=(\alpha,c)\}} = \frac{\int_C \lambda_{\alpha,c}(e,\pi)\, d\pi}{\int_{V_\alpha} \lambda_{\alpha,c}(e,\pi)\, d\pi} \tag{2.1.7}$$

where we have used the obvious relation $P\{J=(\alpha,c)\} = P\{\pi\in V_\alpha, J=(\alpha,c)\}$.

The expression (2.1.7) enable us to interpret the function

$$\beta_{\alpha,c}(e,\pi) := \frac{\lambda_{\alpha,c}(e,\pi)}{\int_{V_\alpha} \lambda_{\alpha,c}(e,\pi)\, d\pi} \tag{2.1.8}$$

as a probability density for the goods produced in an $(\alpha,c)$ jump.

## 2.2 – Generator of the Markov semi group

The object we are interested in is the transition function of the MJP rather than the semi Markov kernel $Q$. The transition function $P_t(e,B)$ gives the conditional

probability to find the system in the Borel set $B \in \mathfrak{B}(E)$ at the time $t$ given that it were in the state $e \in E$ at the time 0.
It is useful to see the transition functions $P_t \quad t \in R_+$ as semi group of operators acting on the Banach space $S$ of the limited, measurable functions on $E$ equipped with the sup norm:

$$\left(P_t u\right)(e) := \int_E P_t\left(e, de'\right) u\left(e'\right) \qquad \forall u \in S \tag{2.2.1}$$

The set of transition functions is called a semi group because they satisfy the semi group property:

$$\begin{aligned} &P_t \circ P_s = P_{t+s} \quad \forall t, s \in R_+ \\ &P_0 = I_S \end{aligned} \tag{2.2.2}$$

where $I_S$ is the identity operator in $S$.

The semi Markov kernel $Q$ and the transition functions $P_t$ are connected through a renewal equation:

$$P_t(e, B) = \int_0^t \int_E Q(e, de', ds) \cdot P_{t-s}(e', B) + \chi_B(e) \cdot \exp\left(-\Lambda(e) t\right) \tag{2.2.3}$$

The equation (2.2.3) can be intuitively obtained decomposing the transition from $e$ into $B$ as a first jump from $e$ to $e' \in E$ taking place at the time $0 \le s \le t$ followed by a transition from $y$ into $B$ during the remaining time $t - s$. The second term in the right hand side of (2.2.3) is the contribution corresponding to no jumps during the time $t$.
The time evolution of the transition function is described also by the Kolmogorov forward equation (KFE):

$$\begin{aligned} &\frac{\partial P_t}{\partial t} = A \circ P_t \\ &P_0 = I_S \end{aligned} \tag{2.2.4}$$

where the operator $A$ acting on $S$ is the generator (infinitesimal transition function) of the semigroup of the MJP.

The renewal equation (2.2.3) can be formally used in order to obtain the infinitesimal transition function $A(e, B)$ defined through a formal Taylor expansion of the transition function for $t = 0$:

$$P_t(e,B) = \chi_B(e) + t \cdot A(e,B) + o(t) \tag{2.2.5}$$

Substituting the (2.2.5) and the (2.1.3) into the (2.2.3) and retaining only the terms up to the first order in $t$ we get the infinitesimal transition function $A$ after a straightforward calculation:

$$A(e,B) = -\Lambda(e)\,\chi_B(e) + \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha} \lambda_{c,\alpha}(e,\pi)\,\chi_B\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi \tag{2.2.6}$$

## 2.3 – The Kolmogorov forward equation

Now we want to prove that the operator (2.2.6) really generate through the KFE (2.2.4) a Markov semi group representing the transition function of the jump process (2.1.3).
The infinitesimal transition function $A$ acts on a function $u \in S$ in the following way:

$$Au(e) = -\Lambda(e)u(e) + \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha} \lambda_{c,\alpha}(e,\pi)\,u\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi \tag{2.3.1}$$

It is easy to show that the operator $A$ is limited and hence continuum in $S$:

$$\begin{aligned}\|Au\| &= \sup\left\{\left|-\Lambda(e)u(e) + \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha} \lambda_{c,\alpha}(e,\pi)\,u\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi\right|, \quad e\in E\right\} \le \\ &\le \sup\left\{\Lambda(e)|u(e)| + \left|\sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha} \lambda_{c,\alpha}(e,\pi)\,u\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi\right|, \quad e\in E\right\} \le 2\Lambda(e)\|u\|\end{aligned} \tag{2.3.2}$$

where we have used the assumption that the function $\Lambda(e)$ is limited (a very reasonable assumption for the intensity of processes in an urban system).

The continuity of $A$ is a sufficient condition for $A$ to generate a semi group of operators $P_t$, $t \in R_+$ in $S$ satisfying the Kolmogorov forward equation (2.2.4).
In order to show that $P_t$ is the kernel of a Markov process in $E$ it remains to prove that the semi group of operators defined through the KFE is positive definite, in the sense that, for every function $u \in S$ such that $u(e) \ge 0 \quad \forall e \in E$ we have $P_t u(e) \ge 0$.
This can be proven writing the solution of the KFE in exponential form:

$$P_t = \exp(At) := \lim_{n\to+\infty}\left(I_S + \frac{t}{n}A\right)^n \tag{2.3.3}$$

Given a positive definite function $u$ we can consider the following sequence of functions $\{u_n\}_{n\in\mathbb{N}}$:

$$u_n = \left(I + \frac{t}{n}A\right)^n u \tag{2.3.4}$$

It is easy to proof that the functions $u_n$ are positive definite for $n$ enough large. Given a generic positive definite function $v \in S$ we have hence:

$$\begin{aligned}&\left(I + \frac{t}{n}A\right)v(e) = v(e) + \frac{t}{n}\left(-\Lambda(e)v(e) + \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha}\lambda_{c,\alpha}(e,\pi)\,v\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi\right) = \\ &\left(1 - \frac{t}{n}\Lambda(e)\right)v(e) + \frac{t}{n}\cdot\sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha}\lambda_{c,\alpha}(e,\pi)\,v\left(\gamma_{c,\alpha}(e,\pi)\right)d\pi\end{aligned} \tag{2.3.5}$$

Let be $\Lambda_0 = \sup_{x\in E}\Lambda(e)$ . Taking $n$ enough large we have that the first term in the (2.3.5) becomes positive: $1 - \frac{t}{n}\Lambda(e) \geq 1 - \frac{t}{n}\Lambda_0 \geq 0$ if and only if $n \geq t\cdot\Lambda_0$.

Thus starting with a positive definite function in (2.3.4) we obtain a sequence of positive definite functions. But we have:

$$P_t u = \lim_{n\to+\infty}\left(I + \frac{t}{n}A\right)^n u = \lim_{n\to+\infty} u_n \tag{2.3.6}$$

That completes the prove because the function $P_t u$ must to be positive definite as limit of positive definite functions.

Up to this point we have proven that the operator $A$ defined by the relation (2.2.6) generates a Markov semi group $P_t$. We have to prove that the related Markov process is exactly the jump process we started with. To show that it is sufficient to express in the renewal equation (2.2.3) the semi Markov kernel $Q$ through the generator $A$ of the semi group:

$$Q(e,B,t) = \frac{1-\exp\left(-\Lambda(e)t\right)}{\Lambda(e)}\left(A(e,B) + \Lambda(e)\chi_B(e)\right) \tag{2.3.7}$$

where we have substitute the (2.2.6) into the (2.1.3). Next we substitute the (2.3.7) in the renewal equation and use the KFE (2.2.4) to express the action of the operator $A$ on the operators $P_t$ of the semi group. After having integrated by part we can check, through a straightforward calculation that the Markov semi group solves the renewal equation.

## 3 – Ordinary differential equations for the mean values of the dynamical variables

Using the KFE it is possible to derive an approximated system of ordinary differential equation for the dynamical variable of the system. Let us start considering a generic measurable real valued function $g : E \to \mathbb{R}$ on the configuration space of the system. Appling both members of the KFE (2.2.4) to $g$ we obtain:

$$\frac{\partial (P_t g)}{\partial t} = (A \circ P_t)\, g \tag{3.1}$$

Using the (2.2.1) and the (2.3.1) to express the action of the operator on $g$ we obtain:

$$\begin{aligned} &\frac{\partial}{\partial t}\int_E P_t(e, de')\, g(e') := \frac{d}{dt}\,\overline{g}_e(t) = \\ &= \int_E P_t(e, de')\left( -\Lambda(e')\, g(e') + \sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha} \lambda_{c,\alpha}(e', \pi)\, g\left(\gamma_{c,\alpha}(e', \pi)\right) d\pi \right) \end{aligned} \tag{3.2}$$

The right hand side of the (3.2) is the time derivative of the mean value $\overline{g}_e(t) = \int_E P_t(e, de')\, g(e')$ of the function $g$ conditioned to the initial configuration $e$.

Let us consider now the equation (3.2) for the function $\omega_{s,j}$ representing the $j$-th component $e_{s,j}$ of the state vector of the cell $s \in \Gamma$: $\omega_{s,j}(e) := e_{s,j}$.
It is easy to specialize the expression $g\left(\gamma_{c,\alpha}(e', \pi)\right)$ appearing in the right hand side of the (3.2) to the functions $\omega_{s,j}$:

$$\omega_{s,j}\left(\gamma_{c,\alpha}(e', \pi)\right) = \omega_{s,j}\left( e' + \sum_{k=1}^{n(\alpha)} \pi_k\, \eta_{c,\alpha}^k \right) = e'_{s,j} + \sum_{k=1}^{n(\alpha)} \pi_k \left(\eta_{c,\alpha}^k\right)_{s,j} \tag{3.3}$$

where $\left(\eta^k_{c,\alpha}\right)_{s,j}$ is the component $j$ of the vector $\eta^k_{c,\alpha}$ in the cell $s$. In the (3.3) we have the (1.1) defining the functions $\gamma_{c,\alpha}$.
Substituting the (3.3) into the (3.29 we obtain:

$$\frac{d\overline{e}_{s,j}}{dt} = -\int_E P_t(e,de')\Lambda(e')e'_{s,j} +$$
$$+\int_E P_t(e,de')\left(\sum_{c\in\Gamma}\sum_{\alpha\in A}\int_{V_\alpha}\lambda_{c,\alpha}(e',\pi)\left(e'_{s,j}+\sum_{k=1}^{n(\alpha)}\pi_k\left(\eta^k_{c,\alpha}\right)_{s,j}\right)d\pi\right) =$$

The last equation can be simplified in the following way:

$$\frac{d\overline{e}_{s,j}}{dt} = -\int_E P_t(e,de')\Lambda(e')e'_{s,j} + \int_E P_t(e,de')e'_{s,j}\sum_{c\in\Gamma}\sum_{\alpha\in A}\lambda_{c,\alpha}(e',\pi) +$$
$$\int_E P_t(e,de')\sum_{c\in\Gamma}\sum_{\alpha\in A}\sum_{k=1}^{n(\alpha)}\pi_k\left(\eta^k_{c,\alpha}\right)_{s,j}\int_{V_\alpha}\lambda_{c,\alpha}(e',\pi)\pi_k\,d\pi$$

Using the definition (2.1.2) of the total intensity we obtain:

$$\frac{d\overline{e}_{s,j}}{dt} = \sum_{c\in\Gamma}\sum_{\alpha\in A}\sum_{k=1}^{n(\alpha)}\left(\eta^k_{c,\alpha}\right)_{s,j}\int_E P_t(e,de')\Pi_{c,\alpha,k}(e') \qquad (3.4)$$

where we have defined

$$\Pi_{c,\alpha,k}(e') := \int_{V_\alpha}\lambda_{c,\alpha}(e',\pi)\pi_k\,d\pi \qquad (3.5)$$

The system of differential equations (3.4) is not of practical use to obtain the time evolution of the mean values of the dynamical variables because it contains the semigroup $P_t$ at the second member.
The case of a deterministic motion of the system along a path $\tilde{\omega}:\mathbb{R}_+\to E$ such that $\tilde{\omega}(0)=e$ corresponds to considering a one parameter set of concentrated measures on $E$ given by $P_t(e,de')=\delta\left(e'-\tilde{\omega}(t)\right)$. Substituting this family of measures $\delta$ in the in (3.4) one obtains the equation:

$$\frac{d\tilde{\omega}_{s,j}}{dt} = \sum_{c\in\Gamma}\sum_{\alpha\in A}\sum_{k=1}^{n(\alpha)}\left(\eta^k_{c,\alpha}\right)_{s,j}\Pi_{c,\alpha,k}(\tilde{\omega}) \qquad (3.6)$$

which is a system of ordinary differential equations for the path $\tilde{\omega}$ and hence for the mean value of the dynamical variables.

In the limit of small variances of the dynamical variables the system (3.6) remains an enough good approximation of the time evolution of the mean value of the dynamical variables.