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The Maximum-Entropy-Based Weight Function in Discrete-Activity-Thermostatted Models

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Abstract: Recently the weighted thermostatted kinetic theory framework with discrete activity has been proposed for modeling the weighted interactions in complex systems. This paper addresses the derivation of the weight function as a solution of an inverse problem based on the macroscopic quantities and specifically on the high-order moments. The weight function, obtained by employing the maximum entropy principle, generalizes the previous published results obtained by employing the zero-order moment.

Keywords: Kinetic Theory, High-order Moment, Inverse Problem, Complexity, Shannon Entropy

1 Introduction

The careful definition of the interactions among the components of a complex system [1] plays a key role in the modeling and simulation of the system. In particular if the complex system consists of a network [2], a weight function needs to be introduced in order to privilegiate and differentiate the most important components that are responsible for the macroscopic (collective) behaviours. Different modeling structures, which have at the base the interaction definitions, e.g. agent-based models [3–8] and the differential equations-based models, have been proposed [9–14].
Recently the thermostatted kinetic theory has been proposed as a general paradigm for the analysis of a complex system [15]. Based on some well-known mathematical structures proposed for the inner matter [16–18], the new thermostatted structures have allowed to enlarge the modeling approach to complex living systems [11, 19–21] even in nonequilibrium conditions (action of an external force field). Accordingly, the complex system is assumed to be composed by active particles which are grouped into different functional subsystems. The interactions among the active particles are modelled by introducing interaction rates and employing the stochastic game theory [22, 23].
In order to better differentiate the interactions, a weight function has been associated to the interaction rate. The derivation of the weight function depends on some constrains (usually the moments of the distribution vector function). In [24] the weight function has been obtained as solution of an inverse problem based on the zero-order moment (the density of the system) and by coupling the methods of the inverse theory [25–28] and the information theory [29–31].
This paper aims to generalize the construction of the weight function proposed in [24] by allowing the definition of inverse problems based on higher-order moments. It is worth stressing that the thermostatted framework includes an operator, called the thermostat operator [32, 33], which allows the conservation of a moment of the system. Accordingly the selected moment, assumed to be the constraint of the system, can be considered as the observed data of the inverse problem. The weight function, obtained by employing the maximum Shannon entropy principle [34–37], allows to generalize the previous published results (see [24]) obtained by assuming the conservation of the zero-order moment.
The present paper is organized into four more sections. In

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detail, after this introduction, the Section 2 deals with the weighted discrete thermostatted framework; the Sections 3 and 4 are devoted to the related inverse problems based on the global and local high-order moments of the system. Section 5 concludes the paper with a critical analysis and applications.

2 The weighted discrete thermostatted kinetic framework

This section is devoted to the basics of the weighted thermostatted kinetic theory that has been recently employed for the analysis of n interacting particle-systems (*functional subsystems*) composing a complex system. An external action $F_i : [0,+\infty[\to \mathbb{R}^+$ acts on the i-th functional subsystem and then the whole system is subjected to the *external force field* $\mathbf{F}(t) = (F_1(t), F_2(t), \ldots, F_n(t))$.
An ith functional subsystem is composed by particles, called active particles, which are able to perform the same strategy $u_i \in \mathbb{R}$, for $i \in \{1,2,\ldots,n\}$. A *distribution function* $f_i(t) := f(t,u_i) : [0,+\infty[\to \mathbb{R}^+$ is introduced in order to describe the time evolution of the ith functional subsystem, for $i \in \{1,2,\ldots,n\}$; in particular $\mathbf{f}(t) = (f_1(t), f_2(t), \ldots, f_n(t))$ denotes the *distribution function vector*. Let $\delta(u-u_i)$ be the delta function centered in u_i, accordingly

$$f(t,u) = \sum_{i=1}^{n} f_i(t)\,\delta(u-u_i)$$

represents the *distribution function* of the overall system.
The *interaction domain* $D^t_{f_h}$ of the functional subsystem f_h represents the set of the functional subsystems which are able, at the time t, to interact with f_h. Accordingly, an interaction function I_{hk} between the functional subsystem f_h and the functional subsystem $f_k \in D^t_{f_h}$ is introduced and assumed factorize as follows:

$$I_{hk}(t) = w_{hk}(t)\eta_{hk}(t),$$

where $\eta_{hk} : [0,+\infty[\to \mathbb{R}^+$ denotes the *interaction rate* and $w_{hk} : [0,+\infty[\to \mathbb{R}^+$ models the weighted interactions (weighted function) and is such that

$$\sum_{k=1}^{n} w_{hk}(t) = 1, \quad \forall h \in \{1,2,\ldots,n\}. \tag{1}$$

Considering the aforementioned parts, the *global weighted pth-order moment* of the system at the time t is defined as follows:

$$\mathbb{E}^w_p[\mathbf{f}](t) = \sum_{h=1}^{n}\sum_{k=1}^{n} u_k^p w_{hk}(t)\, f_k(t), \tag{2}$$

where $\mathbb{E}^w_0[\mathbf{f}]$, $\mathbb{E}^w_1[\mathbf{f}]$ and $\mathbb{E}^w_2[\mathbf{f}]$ denotes the *global weighted density*, the *global weighted linear momentum* and the *global weighted activation energy*, respectively.

In particular the global weighted pth-order moment (2) is the sum of the local weighted pth-order moment of each functional subsystem. Indeed:

$$\mathbb{E}^w_p[\mathbf{f}](t) = \sum_{h=1}^{n}\sum_{k=1}^{n} u_k^p w_{hk}(t)\, f_k(t) = \sum_{h=1}^{n} \mathbb{E}^w_{p,h}[\mathbf{f}](t), \tag{3}$$

where

$$\mathbb{E}^w_{p,h}[\mathbf{f}](t) := \sum_{k=1}^{n} u_k^p w_{hk}\, f_k(t), \quad h \in \{1,2,\ldots,n\}. \tag{4}$$

The *weighted discrete thermostatted kinetic theory framework* reads:

$$\begin{aligned}
&\frac{df_i}{dt}(t) + \sum_{h=1}^{n}\sum_{k=1}^{n}\left(\frac{u_k^p w_{hk}\,(J_k[\mathbf{f}]+F_k) + u_k^p w'_{hk} f_k}{\mathbb{E}^w_p[\mathbf{f}]}\right) f_i \\
&= \sum_{h=1}^{n}\sum_{k=1}^{n} \eta_{hk}\, w_{hk}\, B^i_{hk}\, f_h\, f_k - f_i \sum_{k=1}^{n} \eta_{ik}\, w_{ik}\, f_k + F_i,
\end{aligned} \tag{5}$$

where B^i_{hk} denotes the *transition probability density* that the hth functional subsystem jumps in the ith functional subsystem after the interactions with the kth functional subsystem.

The next sections handle the definition and solution of two inverse problems related to the mathematical framework (5). Specifically the first inverse problem is based on the knowledge of the global weighted pth-order moment (2); the second inverse problem is based on the knowledge of the local weighted pth-order moment (4).
It is worth stressing that the above mentioned inverse problems belong to the class of the *under-determined inverse problems*. Accordingly the definition of further constraints needs to be taken into account in order to ensure the uniqueness of the solution.
Let $\mu = (\mu_1, \mu_2, \ldots, \mu_n) \in \mathbb{R}^n$. The *Shannon entropy* associated to μ is defined as follows [30, 31]:

$$H[\mu] = -\sum_{k=1}^{n} \mu_k \ln \mu_k. \tag{6}$$

In particular the existence of the maximum Shannon entropy principle solution is investigated in the next sections.
In what follows it is assumed that the vector solution $\mathbf{f}$ of the weighted thermostatted framework (5) is composed by continuous functions in the time interval $[0,+\infty[$.

3 The first inverse problem

Let $\mathbf{f}_0$ be a non-negative *initial condition*. The following *inverse problem* is considered:

$$\sum_{h=1}^{n}\sum_{k=1}^{n} u_k^p w_{hk}(t)\, f_k(t) = \mathbb{E}^w_p, \tag{7}$$

where $\mathbb{E}_p^w := \mathbb{E}_p^w[\mathbf{f}_0](t)$ is assumed to be known and $w_{hk}(t)$ is the unknown function.
The weight function w_{hk} is usually assumed to be proportional to the pth-order moment of the particle u_h. Accordingly the function w_{hk} is assumed to factorize as follows:

$$w_{hk}(t) = \mu_k u_h^p f_h(t), \quad h,k \in \{1,2,\dots,n\}, \tag{8}$$

where μ_k is a real constant to be determined according to the constrains. Thus the inverse problem (7) is rewritten, as follows:

$$\begin{aligned} \mathbb{E}_p^w &= \sum_{h=1}^{n}\sum_{k=1}^{n} u_h^p f_h(t)\, u_k^p f_k(t)\, \mu_k \\ &= \sum_{h=1}^{n}\sum_{k=1}^{n} K_{hk}(t)\, \mu_k, \end{aligned} \tag{9}$$

where

$$K_{hk}(t) := u_h^p f_h(t)\, u_k^p f_k(t), \quad \forall h,k \in \{1,2,\dots,n\}. \tag{10}$$

Let $\mathbf{K}[\mathbf{f}](t) = (K_{hk}(t)) \in \mathbb{R}^{n\times n}$. The matrix $\mathbf{K}$ is a symmetric and positive semidefinite matrix. Indeed if $\mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, one has:

$$\begin{aligned} \mathbf{v}\mathbf{K}^t\mathbf{v} &= \left(\sum_{h=1}^{n} v_h u_h^p f_h(t)\right)\left(\sum_{k=1}^{n} v_k u_k^p f_k(t)\right) \\ &= \left(\sum_{h=1}^{n} v_h u_h^p f_h(t)\right)^2 \geq 0. \end{aligned} \tag{11}$$

Moreover, it is easy to prove that if $\mathbb{E}_p^w[\mathbf{f}_0] = n$ then

$$\sum_{k=1}^{n} \mu_k = 1. \tag{12}$$

Bearing all above in mind, the following set of admissible solutions is defined:

$$M_n = \left\{ \mu \in \mathbb{R}^n : \mu_k \geq 0, \sum_{k=1}^{n} \mu_k = 1 \right\}.$$

3.1 The maximum entropy solution

The maximum entropy solution of the inverse problem (9) is the vector μ_H which is solution of the following optimization problem:

$$\mu_H = \arg \max_{\mu \in \mathscr{H}(\mathbf{K}, \mathbb{E}_p^w)} H[\mu], \tag{13}$$

where

$$\mathscr{H}(\mathbf{K}, \mathbb{E}_p^w) := \left\{ \mu \in M_n : \sum_{h=1}^{n}\sum_{k=1}^{n} K_{hk}(t)\, \mu_k = \mathbb{E}_p^w \right\}. \tag{14}$$

Considering all the above, the *lagrangian function* is read, as follows:

$$\begin{aligned} \mathscr{L}[\mathbf{f}](\mu, \lambda_0, \lambda_1) = &- \sum_{j=1}^{n} \mu_j \ln \mu_j - (\lambda_0 - 1)\left(\sum_{j=1}^{n} \mu_j - 1\right) \\ &+ \lambda_1 \left(\mathbb{E}_p^w - \sum_{i=1}^{n}\sum_{j=1}^{n} K_{ij}\mu_j\right), \end{aligned} \tag{15}$$

where $\lambda_0 - 1$ and λ_1 are the *lagrangian multipliers*, and the derivative of the lagrangian function (15) with respect to μ_k, for $k \in \{1,2,\dots,n\}$, is read, as follows:

$$\begin{aligned} \frac{\partial \mathscr{L}}{\partial \mu_k} &= -\frac{\partial}{\partial \mu_k}(\mu_k \ln \mu_k) - (\lambda_0 - 1) \\ &\quad + \lambda_1 \left(-\frac{\partial}{\partial \mu_k}\left(\sum_{i=1}^{n}\sum_{j=1}^{n} K_{ij}\mu_j\right)\right) \\ &= -\ln \mu_k - 1 - (\lambda_0 - 1) - \lambda_1 \sum_{i=1}^{n} K_{ik} \\ &= -\ln \mu_k - \lambda_0 - \lambda_1 \sum_{i=1}^{n} K_{ik}. \end{aligned}$$

Equating to zero and considering the constraints, one has:

$$\exp(\lambda_0) = \sum_{k=1}^{n} \exp\left(-\lambda_1 \sum_{i=1}^{n} K_{ik}\right), \tag{16}$$

and

$$\mu_k = \frac{\exp\left(-\lambda_1 \sum_{i=1}^{n} K_{ik}\right)}{\exp(\lambda_0)} = \frac{\exp\left(-\lambda_1 \sum_{i=1}^{n} K_{ik}\right)}{\sum_{k=1}^{n} \exp\left(-\lambda_1 \sum_{i=1}^{n} K_{ik}\right)}. \tag{17}$$

Accordingly, the maximum entropy principle solution of the inverse problem (9) is read, as follows:

$$w_{hk}(t) = \frac{u_h^p \exp\left(-\lambda_1 u_k^p f_k(t) \sum_{i=1}^{n} u_i^p f_i(t)\right)}{\sum_{k=1}^{n} \exp\left(-\lambda_1 u_k^p f_k(t) \sum_{i=1}^{n} u_i^p f_i(t)\right)} f_h(t), \tag{18}$$

where the Lagrange multiplier λ_1 is solution of the following nonlinear equation:

$$-\frac{\partial}{\partial \lambda_1} \ln \sum_{k=1}^{n} \exp\left(-\lambda_1 u_k^p f_k(t) \sum_{i=1}^{n} u_i^p f_i(t)\right) = \mathbb{E}_p^w.$$

4 The second inverse problem

Let $\mathbf{f}_0$ be a non-negative *initial condition*. The following *inverse problem* is now considered:

$$\sum_{k=1}^{n} u_k^p w_{hk}(t) f_k(t) = \mathbb{E}_{p,h}^w, \qquad (19)$$

where $\mathbb{E}_{p,h}^w := \mathbb{E}_{p,h}^w[\mathbf{f}_0](t)$, for $h \in \{1,2,\dots,n\}$, is assumed to be known and $w_{hk}(t)$ is the unknown function. As in the last section, the weight function w_{hk}, for $h,k \in \{1,2,\dots,n\}$, is assumed to factorize as follows:

$$w_{hk}(t) = u_h^p \mu_k f_h(t), \quad \mu_k \in \mathbb{R}, \qquad (20)$$

where now μ_k is the unknown constant to be determined. Thus the inverse problem (19) is rewritten, as follows:

$$\sum_{k=1}^{n} \left(u_h^p f_h(t) u_k^p f_k(t)\right) \mu_k = \mathbb{E}_{p,h}^w, \quad h \in \{1,2,\dots,n\}. \quad (21)$$

Hence the vectorial form of the inverse problem (21) is written, as follows:

$$\mathbf{K}[\mathbf{f}](t)\,\mu = \bar{\mathbb{E}}_p^w, \qquad (22)$$

where $\bar{\mathbb{E}}_p^w = \left(\mathbb{E}_{p,1}^w, \mathbb{E}_{p,2}^w, \dots, \mathbb{E}_{p,n}^w\right)$, $\mu = (\mu_1, \mu_2, \dots, \mu_n) \in \mathbb{R}^n$, and $\mathbf{K}[\mathbf{f}](t) = (K_{hk}(t)) \in \mathbb{R}^{n\times n}$ is the matrix (10).
As in the previous section, if it is assumed that $\mathbb{E}_{p,h}^w(t) = 1$, it is easy to prove that

$$\sum_{k=1}^{n} \mu_k = 1.$$

*Remark.*If the inverse matrix of $\mathbf{K}[\mathbf{f}](t)$ exists, then

$$w_{hk}(t) = \left(\sum_{l=1}^{n} K_{kl}^{-1}(t)\,\mathbb{E}_{p,l}^w\right) u_h^p f_h(t), \qquad (23)$$

where $\mathbf{K}^{-1}[\mathbf{f}](t) = (K_{kl}^{-1}(t))$ denotes the inverse matrix of $\mathbf{K}[\mathbf{f}](t)$. It easy to see that the existence of the inverse matrix is ensured if $\mathscr{F} = \{f_1(t), f_2(t), \dots, f_n(t)\}$ is a set of linearly independent functions.

4.1 The maximum entropy solution

As in the previous section, the following *optimization problem* is established:

$$\mu_H = \arg \max_{\mu \in \mathscr{H}(\mathbf{K}, \bar{\mathbb{E}}_p^w)} H[\mu], \qquad (24)$$

where

$$\mathscr{H}(\mathbf{K}, \bar{\mathbb{E}}_p^w) := \left\{\mu \in M_n : \mathbf{K}[\mathbf{f}](t)\,\mu = \bar{\mathbb{E}}_p^w\right\}. \qquad (25)$$

The related *Lagrangian function* $\mathscr{L}$ thus reads:

$$\begin{aligned}
&\mathscr{L}[\mathbf{f}](\mu, \lambda_0, \lambda_1, \lambda_2, \dots, \lambda_n) = \\
&\quad -\sum_{j=1}^{n} \mu_j \ln \mu_j - (\lambda_0 - 1)\left(\sum_{j=1}^{n} \mu_j - 1\right) \\
&\quad + \sum_{i=1}^{n} \lambda_i \left(\mathbb{E}_{p,i}^w - \sum_{j=1}^{n} K_{ij}\mu_j\right),
\end{aligned}$$

where $\lambda_0 - 1$ and λ_i, for $i \in \{1,2,\dots,n\}$, denote the related *lagrangian multipliers*.
The related derivative of the lagrangian function with respect to μ_k writes:

$$\begin{aligned}
\frac{\partial \mathscr{L}}{\partial \mu_k} &= -\frac{\partial}{\partial \mu_k}\left(\sum_{j=1}^{n} \mu_j \ln \mu_j\right) - (\lambda_0 - 1)\frac{\partial}{\partial \mu_k}\left(\sum_{j=1}^{n} \mu_j - 1\right) \\
&+ \sum_{i=1}^{n} \lambda_i \frac{\partial}{\partial \mu_k}\left(\mathbb{E}_{p,i}^w - \sum_{j=1}^{n} K_{ij}\mu_j\right) \\
&= -\ln \mu_k - \lambda_0 - \sum_{i=1}^{n} \lambda_i K_{ik}.
\end{aligned}$$

Considering the previous section, one knows that the maximum entropy principle solution $w_{hk}(t)$, for $h,k \in \{1,2,\dots,n\}$, of the inverse problem (22) is read, as follows:

$$w_{hk}(t) = \frac{u_h^p \exp\left(-u_k^p f_k(t) \sum_{i=1}^{n} \lambda_i u_i^p f_i(t)\right)}{\sum_{k=1}^{n} \exp\left(-u_k^p f_k(t) \sum_{i=1}^{n} \lambda_i u_i^p f_i(t)\right)} f_h(t), \quad (26)$$

where the vector $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_n) \in \mathbb{R}_+^n$ is solution of the following nonlinear vectorial equation:

$$-\nabla_\lambda \ln \sum_{k=1}^{n} \exp\left(-u_k^p f_k(t) \sum_{i=1}^{n} \lambda_i u_i^p f_i(t)\right) = \mathbb{E}_p^w.$$

5 Conclusion and perspectives

The generalization of the results published in [24] has been the main objective of the present paper. Specifically the main aim is the definition of a robust mathematical modeling theory which is able to adapt the interactions of the active components of a complex system during its natural or constrained evolution. According to the results of [24] and of the present paper, the natural constraints are established by the moments of the distribution vector function (e.g. density and activation energy). The important advantage of the approach proposed in the present paper is the possibility to link the microscopic behavior (the interactions) to the macroscopic behavior thus allowing the definition of a multiscale approach. However, depending on the complex system under consideration, knowledge of such a moment can be a complicated issue and only some previsions of their time evolution can be conjectured. This evolution is, for instance, assumed in some living systems, such as in biological and human behavior systems (crowds, vehicular traffic) where the first-order moment or the activation energy can be assumed to follow a stochastic process. From the theoretical viewpoint, the inverse problem has been resolved by employing the most famous entropy principle of Shannon. Although the Shannon entropy is considered an optimal function, other entropy functions can be employed in an attempt to better optimize the role and the rules of the interactions [38–41].

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