SOME DYNAMIC EFFECTS OF THE AGGREGATION OF GENERIC MODEL SYSTEMS - THE MASTER EQUATION APPROACH

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ABSTRACT

The relationship between the dynamic behavior of individual components of a large system and the overall behavior of the large system has rarely been analyzed in the system dynamics literature. The usual approach is to treat the large system (e.g., a national economy) as a lumped-parameter version of the component systems.

A number of examples from physical systems (plasma instabilities, fluid and chemical-reaction waves) suggest that the lumped parameter approach is not always adequate as a representation of the dynamics of systems or as a cogent explanation of the behavior of aggregate systems. In particular, new collective modes of behavior are found when the stochastic distribution of micro-level systems over internal states is considered. The proper treatment of the aggregation of micro-systems can reveal novel dynamic behavior modes and can indicate under what conditions these modes may become active. The explicit treatment of the aggregation of micro-systems can also clarify the relationships between the structure and parameters of the micro-systems and those of a lumped-parameter representation of the macro-system, thus giving some precision to arguments based on macro-level models of interacting micro-level systems.

One approach to the study of the collective behavior of elementary systems uses the concept of a "dissipative structure" as developed by Prigogine and colleagues over the past fifteen years. This paper continues the work of a previous paper on the subject by applying the Master Equation Formulation to several generic models of first and second order (including delays, sigmoid growth, predator-prey and other oscillatory systems). Conditions under which novel aggregate behavior may be expected to appear are determined. Since linear systems do not present any novelty in the theory, most attention is focused on non-linear examples.

INTRODUCTION

In a previous paper (1), an adaptation of system dynamics modeling was proposed in order to deal explicitly with the question of aggregation of diverse but similar units. The approach used was based on a model of the stochastic nature of interactions in a system leading to the derivation of a Master Equation for the joint probability distribution of level variables. Inspired by recent results in the literature of non-equilibrium thermodynamics and chemical kinetics (2, 3, 4), the analysis of a first-order delay and the development of a consistent treatment of equations for the most-probable evolution of the system and for the mean and variance of fluctuations about this path were presented. The present paper applies the same methods of analysis to three generic models: a logistic growth model, a two-level inventory-workforce model and a predator-prey model. This set includes two examples of non-linear systems and two examples of oscillatory systems. The set includes small structures often found in larger models and often used for demonstrating dynamic principles. The analysis of these models goes some way to completing the research program proposed in the above-mentioned paper and provides some insight into the effects of stochasticity in dynamic systems.

The results of the analysis of these three models can be summarized briefly as follows. To lowest order in the expansion scheme used, the fluctuations behave similarly to the macroscopic system. For example, in linear systems the eigenvalues of the fluctuation equation are the same as for the most-probable path and for non-linear systems the fluctuation distribution changes with the evolution of the macroscopic system in a not-too-surprising manner - the variance grows or contracts during periods of expansion or
decline and stabilizes if the macroscopic system reaches equilibrium. Based on a small number of cases, these results are not perfectly general; however they are consistent with results from the scientific literature referenced above.

LOGISTIC GROWTH

The logistic growth model is an example of a one-level, two-loop, non-linear system in which the dominance of one loop over another changes as the initial growth stage is replaced by an adjustment to equilibrium. This model is used to describe the growth of a population limited by external constraints (area, food supply, ...). In differential equation form, as shown in equation (1), we take the saturation limit to be \( X \) and introduce the growth parameter, \( a \).

The event-probability table, Table 1, describes the Markovian, stochastic model in terms of the probability of the events, \( dx \), which change the size of the population in a short time interval, \( dt \). The probability of an event depends on the nature of the event (the value of \( dx \)) and on the probability, \( P(x,t) \), that the system is in a given state, \( x \), at a time, \( t \).

The Master Equation for \( P \) is shown in equation (2)

\[
\frac{dP}{dt} = aX(x-1)P(x-1,t) - aXP(x,t) + a(x+1)^2P(x+1,t) - ax^2P(x,t)
\]  
(2)

An alternative form of the Master Equation is given in equation (3) where \( w(x, dx) \) is the transition probability per unit time, describing the rate of increase or decrease of the state probability, \( P \).

\[
\frac{dP}{dt} = \int dx w(x, dx)P(x- dx, t) - w(x, dx)P(x, t)
\]  
(3)

For discrete changes in state, the integral becomes a sum and we can specify the stochastic model in a table of transition probabilities as shown in Table 2.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Probability, ( w(x, dx) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( dx = 1 )</td>
<td>( ax )</td>
</tr>
<tr>
<td>( dx = -1 )</td>
<td>( ax^2 )</td>
</tr>
</tbody>
</table>

Table 2: Logistic model transition probabilities

A consistent expansion of the Master Equation in terms of a parameter, \( \Omega \), representing the size of the system compared to the stochastic fluctuations, leads to consideration of the equations for the evolution of the most-probable state, \( y \), and for fluctuations, \( \delta y \), about this state (1). These equations involve the moments of the transition probability distribution and are summarized in equation (3) for the general case.
\[
\begin{align*}
dy/dt &= c_i(y) \\
d\delta y/dt &= K(y) y \\
d y/dt &= K\alpha + 1/2 K'\sigma \\
d\sigma/dt &= K\sigma + (K\sigma)^2 + D
\end{align*}
\]

In general, \( y \) is a state vector, \( \delta y \) a fluctuation vector with mean, \( \mu \), and covariance matrix, \( \sigma \), and the function \( c_i \) is a vector function of \( y \) while the functions \( K \) and \( D \) are matrix functions of the state, \( y \). In terms of the transition probability, we have the following expressions for \( c_i, K \) and \( D \).

\[
\begin{align*}
c_i(y) &= \int \delta x w(y, \delta x) \delta x \\
K_{ij}(y) &= \frac{dc_i(y)}{dy_j} \\
D_{ij}(y) &= c_{ij}^{1j}(y) = \int \delta x w(y, \delta x) (\delta x)^2
\end{align*}
\]

For the logistic growth model, we find

\[
\begin{align*}
c_i(y) &= ay(x-y) \\
K &= a(x-2y) \\
D &= ax^2 + ay^2
\end{align*}
\]

Thus we recover, to lowest order in the expansion, the original macroscopic or deterministic equation. The stochastic model permits us to specify the equations of evolution of the mean and variance of fluctuations, namely

\[
\begin{align*}
d\mu/dt &= a(x-2y)\mu - a\sigma \\
d\sigma/dt &= 2a(x-2y)\sigma + ay(x+y)
\end{align*}
\]

From these equations we note that for \( y = x/2 \) initially, the mean and variance of fluctuations grow quasi-exponentially, while as \( y \) approaches the macroscopic saturation limit, \( x \), the mean of fluctuations decreases to \(-1\) and the variance approaches the equilibrium value of \( x \). The Markovian assumption for the transition probabilities gives in this limit an almost-Poisson distribution whose mean is \( x-1 \) and variance \( x \). As seen from equation (6), the variance passes from an initial growth phase to a final equilibrium, a behavior noted by Kubo et al. (7) in relation to a chemical reaction model.

**INVENTORY-WORKFORCE MODEL**

This two-level model is a linear model of a commonly occurring situation in which the delays inherent in managing a resource (the workforce, \( L \)) to achieve some desired level of performance (measured by a stock of finished goods, \( S \)) in the face of external influences (the sales rate, \( SALES \)), leads to oscillations as the system adjusts to a new equilibrium after a step change in \( SALES \). The differential form of this model in terms of the above variables is given in equation (7)

\[
\begin{align*}
dL/dt &= (DL - L)/TAL \\
dS/dt &= PROD*SALES - PROD - \text{SALES} \quad (7) \\
DL &= (DS - S)/(TAS*PROD) \\
DS &= SCOV*SALES
\end{align*}
\]

where

\[
\begin{align*}
TAL, TAS &= \text{Time to adjust workforce, stock (weeks)} \\
PROD &= \text{Productivity (un/man)/week} \\
SCOV &= \text{Stock coverage time (weeks)}
\end{align*}
\]
In a more compact, abstract form we can write

\[
\begin{align*}
\frac{dx_1}{dt} &= -a_{11}x_1 - a_{12}x_2 + b_1u \\
\frac{dx_2}{dt} &= a_{21}x_1 - u
\end{align*}
\]

where

\[
\begin{align*}
a_{11} &= -1/TAL \\
a_{12} &= 1/(TAS*TAL*PROD) \\
a_{21} &= PROD \\
b_1 &= SCOV/(TAS*PROD)
\end{align*}
\]

A transition probability table for this model is shown in Table 2, where \( x = (x_1, x_2) \)

<table>
<thead>
<tr>
<th>Transition</th>
<th>Probability w(x, x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta x_1 = 1, \delta x_2 = 0 )</td>
<td>( b_1u )</td>
</tr>
<tr>
<td>( \delta x_1 = 1, \delta x_2 = 0 )</td>
<td>( a_{11}x_1 + a_{12}x_2 )</td>
</tr>
<tr>
<td>( \delta x_1 = 0, \delta x_2 = 1 )</td>
<td>( a_{21}x_1 )</td>
</tr>
<tr>
<td>( \delta x_1 = 0, \delta x_2 = 1 )</td>
<td>( u )</td>
</tr>
</tbody>
</table>

Table 2: Inventory-Workforce Model - Transition Probabilities

We remark, for future reference, that the transitions \( \delta x_1 = 1 \) and \( \delta x_2 = 1 \) are assumed independent of each other.

The first and second moments of the transition probability distribution are shown in equation (9)

\[
c_1(x) = \begin{pmatrix} -a_{11}x_1 + a_{12}x_2 + b_1u \\ a_{21}x_1 - u \end{pmatrix}
\]

\[
c_2(x) = \begin{pmatrix} a_{11}x_1 + a_{12}x_2 + b_1u & 0 \\ 0 & a_{21}x_1 + u \end{pmatrix}
\]

The independence of the transitions \( \delta x_1 = 1, \delta x_2 = 1 \) leads to the second moment matrix, \( c_2 \), being diagonal. The equations of evolution of the most probable state, \( x \), are the same as the deterministic equations, that is

\[
\frac{dx}{dt} = c_1(x)
\]

The equations of evolution of the mean and variance of fluctuations about this state are determined by substituting for \( K \) and \( D \) in equation (3) where

\[
K = \begin{pmatrix} -a_{11} & -a_{12} \\ a_{21} & 0 \end{pmatrix}
\]

\[
D = c_2(x)
\]

Thus for this linear model, the autonomous part of the equations of evolution of the fluctuations and of the mean are the same as for the deterministic system. Hence the dynamic characteristics (damping, oscillation frequency, ...) summarized by the eigenvalues of \( K \) are the same as for the deterministic model. We note that the eigenvalues, \( \lambda_{1,2} \), are given by
\[ \lambda_{1,2} = a_{11} \pm \left( a_{11}^2 - 4a_{12}a_{21} \right)^{\frac{1}{2}} \]

and these give exponential decay, with or without oscillations. The equations for the components of the covariance matrix can be written by rearranging the corresponding component of equation (3), namely

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{12} \\
\sigma_{22}
\end{pmatrix}
= \begin{pmatrix}
-2a_{11} & -2a_{12} & 0 \\
a & -a & -a \\
0 & 2a_{21} & 2a_{21}
\end{pmatrix}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{12} \\
\sigma_{22}
\end{pmatrix}
+ \begin{pmatrix}
a_{11}x_1 & -a_{12}x_2 \\
a_{11}x_1 & 0 \\
a_{21}x_2 & -a_{21}x_1 + u
\end{pmatrix}
\] (13)

The eigenvalues of this equation are

\[ \lambda_0 = -a_{11}, \lambda_{1,2} = -a_{11} \pm \left( a_{11}^2 - 4a_{12}a_{21} \right)^{\frac{1}{2}} \] (14)

Thus the covariance components decay exponentially with or without oscillations under the same conditions as the deterministic model. This is a general result for linear systems which follows from the fact that the derived matrix, \( \mathbf{K} \), for a linear system, is identical to the system matrix.

**Lotka–Volterra Model**

This two-level, non-linear model of interactions between two populations (predator and prey) has also been used to study bi-molecular chemical reactions. The generalization to more than two species has been treated elsewhere (5). Our interest in this model stems from the fact that it generates non-linear oscillations and hence combines the features of the models discussed previously. The differential equation form of the model is shown in equation (16) where \( x_1 \) is the number of "prey" and \( x_2 \) is the number of "predators":

\[
\begin{align*}
dx_1 &= ax_1 - bx_1x_2 \\
dx_2 &= bx_1x_2 - dx_2
\end{align*}
\] (15)

A transition probability table for this system is shown in Table 3.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Probability ( w(x, \delta x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta x_1 = +1, \delta x_2 = 0 )</td>
<td>( ax_1 )</td>
</tr>
<tr>
<td>( \delta x_1 = -1, \delta x_2 = +1 )</td>
<td>( bx_1x_2 )</td>
</tr>
<tr>
<td>( \delta x_1 = 0, \delta x_2 = -1 )</td>
<td>( dx_2 )</td>
</tr>
</tbody>
</table>

Table 3: Lotka–Volterra Model Transition Probabilities

In this model, the assumption is made that the reduction of the component \( x_1 \) by one unit is simultaneous with the increase by one unit of the component \( x_2 \). While the assumption is not very realistic for predator-prey models, it
is an accurate representation of chemical reactions. We retain this assumption for comparison with the inventory-workforce model where the corresponding changes in levels are independent.

The first moment of the fluctuations about the most-probable path gives an equation which is the same as equation (15). The second moment permits us to determine the evolution of the variance from the equation

\[
\frac{d}{dt} \begin{pmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{22} \end{pmatrix} = \begin{pmatrix} 2(a - bx_2) & -2bx_1 & 0 \\ bx_2 & (a - bx_2 + bx_1 - d) - bx_1 & 0 \\ 0 & 2bx_2 & 2(bx_1 - d) \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{22} \end{pmatrix} + \begin{pmatrix} bx_1 + bx_2 \\ bx_1 \\ b x_1 x_2 \end{pmatrix}
\]

The simultaneous increase and decrease of the two components, \( x_1, x_2 \), shows up as the non-autonomous term in the equation for \( \sigma_{12} \).

During periods when the levels are slowly changing, approximate eigenvalues of the autonomous part of equation (16) can be found. These eigenvalues are

\[
\lambda_{1,2} = (g_1 + g_2) \pm ((g_1 - g_2)^2 - 8d_1d_2)^{1/2}; \quad \lambda_0 = g_1 + g_2
\]

where

\[
\begin{align*}
    g_1 &= a - bx_2, \text{ "growth rate" of } x_1 \\
    g_2 &= bx_1 - d, \text{ "growth rate" of } x_2 \\
    d_1 &= bx_2, \text{ interaction of } x_2 \text{ on } x_1 \\
    d_2 &= bx_1, \text{ interaction of } x_1 \text{ on } x_2
\end{align*}
\]

The first pair of eigenvalues are almost the same as the approximate eigenvalues of the most-probable path, namely

\[
2 \lambda_{1,2} = (g_1 + g_2) + ((g_1 - g_2)^2 - 4d_1d_2)^{1/2}
\]

The similarity with the inventory-workforce results is remarkable in light of the different underlying stochastic models.

Although a general solution of equations (15) and (16) is not available, a special case corresponding to simultaneous growth or decline of both populations gives a result similar in spirit to the growth of the variance in the logistic model. When \( g_1 = g_2 = g \), the equations for \( \sigma_{11} \) and \( \sigma_{22} \) may be combined and integrated assuming \( x_1, x_2 \) are constant (or very slowly changing). The result, with initial values \( \sigma_{11} = \sigma_{22} = 0 \) for convenience, is

\[
x_2 \sigma_{11} + x_1 \sigma_{22} = A(x_1, x_2) (e^{2gt} - 1)/2g
\]

The linear combination of variances is positive (as it should be) and grows or declines according as \( g \) is greater or less than zero.

**Comments**

From these examples we see that in the linear case, the stochastic model introduces no novel behavior compared to the deterministic approach, i.e. the eigenvalues of the fluctuation distribution are the same as those of the macroscopic deterministic model. For non-linear models, the fluctuations may show behavior similar but not identical to the macroscopic system.

The specification of a model for the fluctuations should be of some use in identifying a macroscopic model. However the results of the (approximate) eigenvalue calculations for the two oscillatory models indicated a certain 'robustness' of the eigenvalues in the face of alternative stochastic models.
That is, the differences in the 'eigenvalues' of the macroscopic and the fluctuation equations is due to structural factors, such as the number and polarity of minor loops, and not to the detailed differences in assumptions about the simultaneity or independence of some of the stochastic events underlying the dynamics. This means that such dynamic characteristics as eigenvalues are not the best instruments for specifying a model and that other instruments must be used.

One possibility for further investigation rests on the observation that in some regions of state space or over some time-interval, the assumption of slowly-varying states may break down and a more detailed study of the transition may reveal non-exponential time behavior which is characteristic of the stochastic model. Such is the case for the logistic model where the increase in the variance during the growth period may be of several orders of magnitude according to the first-order model while a more detailed analysis reveals slower than exponential time-variation in the transition from growth to equilibrium-seeking (6). Further work on other generic models needs to be done to verify if the increase in variance (or flattening of the distribution) is evident in other, non-linear systems. Informal tests on the 'Market Growth' model are as yet inconclusive on this point.

Extensions of the Master Equation

The models presented here are for systems that are uniform in space. The diffusion term, D, in equation (3), represents a diffusion rate in the space of level variables and as such establishes a scale factor for the variance as seen, for example in equation (17). To study the effects of diffusion into and out of the system, the master equation can be modified to account for arrivals and departures across some boundary. Such a modification contributes terms similar to linear, delay-type terms in the macroscopic model. The interpretation of these terms as diffusive introduces measures of the critical 'size' of a system necessary to support instability (6).

Thus, it appears that the state-space diffusion term, D, cannot explain the onset of instability, contrary to a claim made in a previous paper (1). However, by the same token, it appears that the relationship between delay and diffusion-type terms may lead to a specification of critical delay-times which give rise to instability, or whose control can suppress instability. Analysis along these lines is being pursued.
References


