Compositional evolution with mass transfer in closed systems

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Abstract

Evolution of compositions in time, space, temperature or other covariates is frequent in practice. For instance, the radioactive decomposition of a sample changes its composition with time. Some of the involved isotopes decompose into other isotopes of the sample, thus producing a transfer of mass from some components to other ones, but preserving the total mass present in the system. This evolution is traditionally modelled as a system of ordinary differential equations of the mass of each component. However, this kind of evolution can be decomposed into a compositional change, expressed in terms of simplicial derivatives, and a mass evolution (constant in this example). A first result is that the simplicial system of differential equations is non-linear, despite of some subcompositions behaving linearly.

The goal is to study the characteristics of such simplicial systems of differential equations such as linearity and stability. This is performed extracting the compositional differential equations from the mass equations. Then, simplicial derivatives are expressed in coordinates of the simplex, thus reducing the problem to the standard theory of systems of differential equations, including stability. The characterisation of stability of these non-linear systems relays on the linearisation of the system of differential equations at the stationary point, if any. The eigenvelues of the linearised matrix and the associated behaviour of the orbits are the main tools. For a three component system, these orbits can be plotted both in coordinates of the simplex or in a ternary diagram. A characterisation of processes with transfer of mass in closed systems in terms of stability is thus concluded. Two examples are presented for illustration, one of them is a radioactive decay.

Key words: balance, simplex, Aitchison geometry, orthonormal basis, stability, ordinary differential equations, stationary point, radioactive decay.

1 Introduction

In many practical situations a composition may evolve with some covariates like time, space, temperature or pressure. Many cases can be described as a mixture of different mass species; each species gaining or losing mass and possibly transferring the lost mass to other species. When a single covariate (e.g. evolution in time) is considered, continuous evolution is frequently described using ordinary differential equations (ODE) or systems of them, where the unknown functions are the evolution of the mass of each species with respect to the covariate.

Many examples can be found. For instance, a radioactive sample containing a given mass of three different isotopes. The first isotope, when disintegrates, becomes the second; and the second one disintegrates into the third, being the latter one inert. This encloses (a) evolution in time of the total mass (e.g. constant; decreasing because some residual material is not in the system, etc.); and (b) evolution of concentration of isotopes which constitutes the compositional process. This process may be considered deterministic because its variability is very small.

Another typical example is the evolution of a population categorised into age groups and sex. In time, each category gains individuals from younger classes (deterministically), loses individuals by death and gains or loses by migration. Again there is an evolution of the total population and the change of the composition of such a population irrespective of the total population.

This study is focussed on closed systems in which the total mass is constant in time and the masses are gained or lost proportionally to the present mass of each species or component. For D mass species the system of ODE can be written as

$$\frac{d}{dt}\mathbf{N}(t) = A\ \mathbf{N}(t) + \mathbf{f}(t)\ , \tag{1}$$

where $\mathbf{N}(t)$ is a D-column-vector with positive functions $N_i(t)$ as components; $A = (\alpha^i_j)$ is a square D-matrix controlling loss and growth of each component; and $\mathbf{f}(t)$ is a forced input-output flow of mass. The simplest example occurs when matrix A is diagonal and $\mathbf{f}(t) = 0$. This corresponds to exponential growth (decay) of each mass without interaction (disintegration without transfer of mass, growth of bacteria without interaction). Whenever A is not diagonal, there is some transfer of mass between components. The mass process admits a number of representations. The obvious one is component-wise matching the component representation of $\mathbf{N}(t)$. The separation of the compositional part of $\mathbf{N}(t)$ from the total mass is also an intuitive representation $\mathbf{N}(t) = M(t) \cdot \mathbf{x}(t)^t$, where $M(t) = \sum_{i=1}^{D} N_i(t)$ and $\mathbf{x}(t) = \mathcal{C}\mathbf{N}(t)^t$, being $\mathcal{C}$ the closure operator so that the components of $\mathbf{x}(t)$ add to a fixed constant (here assumed to be 1). Other representations are possible, for instance, the compositional part $\mathbf{x}(t)$ and $N_1(t)$ also fully describe the mass process. The case with diagonal A has been studied from the compositional point of view in Egozcue et al. (2003); Egozcue and Pawlowsky-Glahn (2005). It is the paradigm of a linear process in the simplex: the orbit is a straight-line in the simplex.

A mathematical and practical question concerns to the character of the equations describing the mass process when compared to their compositional representation. A first inspection reveals that the linear or non-liner character may be reversed from the mass to the compositional part and viceversa. Also the stability may change. These changes can be illustrated with a simple example using the well-known Verhulst (1838) logistic equation that, being non-linear, has a compositional part just linear. Furthermore, the logistic equation, as a mass evolution, is stable, and its compositional part is unstable. To show these facts, consider a large number of resource cells M. These cells may be occupied by an individual of a population; let this number of cells be N_1, $N_1 \leq M$. The population model was proposed to be

$$\frac{d}{dt}N_1 = \frac{r}{M}\ N_1\ (M - N_1)\ , \tag{2}$$

whose solution is the also well-known logistic curve or sigmoid,

$$N_1(t) = \frac{MN_1(0)\exp(rt)}{M + N_1(0)(\exp(rt) - 1)}\ .$$

The complementary of N_1 is $N_2 = M - N_1$. A substitution in (2) gives a second differential equation for N_2, equal to (2) up to a sign. Equation (2) is typically non-linear, a Riccati equation; and typically stable because the solution remains bounded. In order to study the compositional part of this simple equation, (N_1, N_2) can be divided by the constant total mass M thus obtaining the same equations just substituting N_i by $x_i = N_i/M$. To build up compositional derivatives (see Appendix B), each equation is divided by the variable to get a logarithmic derivative and then exponentials are taken:

$$\exp \frac{d}{dt} \log x_1 = (\exp(x_2))^{r/M} \ , \ \exp \frac{d}{dt} \log x_2 = (\exp(x_1))^{-r/M} \ ,$$

and after closure

$$D^{\oplus}\mathbf{x} = \mathcal{C}[(\exp x_2)^{r/M}, (\exp x_1)^{-r/M}] \ .$$

The equation of the only coordinate, x^*, of the composition $\mathbf{x}$ becomes

$$\frac{d}{dt} x^* = \frac{r}{\sqrt{2}}(x_1 + x_2) = \frac{r}{\sqrt{2}} \ ,$$

which is simple and linear, and moreover, unbounded because x^* grows indefinitely in time. In fact, the solutions in the only coordinate and in the simplex are

$$x^* = x_0^* + \frac{rt}{\sqrt{2}} \quad , \quad \mathbf{x} = \mathbf{x}_0 \oplus \left(t \odot \mathcal{C} \left(\exp \left[\frac{r}{\sqrt{2}}, \frac{-r}{\sqrt{2}} \right] \right) \right) \ ,$$

which represents a straight-line in the plane (t, x^*) and in the simplex. After this unexpected situation of change of character of the compositional part of a simple equation, one should ask for the behaviour of the compositional part of a linear system of differential equations like (1) representing a mass evolution.

A further reason to study the compositional part of a mass evolution is that the total mass process is seldom observed or it is irrelevant and the compositional part is the only model information that is actually useful. Here closed systems are considered, with $M(t)$ constant and $\mathbf{f}(t) = 0$. The goal is to study the stability of the compositional process depending on the coefficients in A. Unstable processes tend to extinction of some species (singular compositions placed at infinity). Stable compositional processes produce stationary cycles or converge to a fixed composition. This study requires to derive the compositional differential equations of (1), which are non-linear in the simplex. However, stability can be studied using Lyapunov techniques which involve the linearisation of the system. Finally, the linear system is transformed into orthogonal coordinates where the standard theory of systems of ODE's applies.

2 Compositional equations of a closed system

Consider the homogeneous linear system of D ODE's corresponding to (1)

$$\frac{d}{dt}\mathbf{N}(t) = A \ \mathbf{N}(t) \ , \ N_i(t) > 0 \ , \ i = 1, 2, \ldots, D \ , \qquad (3)$$

which represents the time-evolution of the mass of D species (Moral and Pacheco, 2003). Dependence of functions with respect to time is suppressed when it is not needed for interpretation.

Definition. *A dynamical system such as (3) is called a closed system, if the sum* $M = \sum_{i=1}^{D} N_i$ *is constant.*

The system (3) is a closed system if, and only if, the column-wise addition the coefficients of matrix system is zero, i.e.

$$\sum_{i=1}^{D} \alpha_j^i = 0 \ , \ j = 1, 2, \ldots, D \ . \qquad (4)$$

A consequence is that the sum of all entries of A is null.

Assume that the system (3) is a closed system. The species can be described as proportions of the total mass $\mathbf{x} = M^{-1}\mathbf{N}^t$, where the vector of proportions is considered a row-vector as commonly done in compositional data analysis. With this notation the system (3) is rewritten

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{x}(t)\ A^t\ ,\ \mathbf{x} = (x_1, x_2, \ldots, x_D) \in \mathcal{S}^D\ , \tag{5}$$

where $\mathcal{S}^D$ is the unit simplex of D parts (its dimension as vector space is $D-1$). The equations of the system (5) can be rewritten as logarithmic derivatives,

$$y_i = \frac{d}{dt}\log x_i = \frac{1}{x_i}\frac{dx_i}{dt} = \alpha_1^i\frac{x_1}{x_i} + \alpha_2^i\frac{x_2}{x_i} + \cdots + \alpha_D^i\frac{x_D}{x_i}\ ,\ i = 1, 2, \ldots, D\ . \tag{6}$$

Arranging the differential equations (6) in a row-vector and closing them to unit,

$$D^{\oplus}\mathbf{x} = \mathcal{C}\exp\left(\frac{d}{dt}\log\mathbf{x}\right) = \mathcal{C}\exp(\mathbf{y})\ ,\ \mathbf{y} = (y_1, y_2, \ldots, y_D)\ , \tag{7}$$

where $D^{\oplus}$ is the ordinary derivative with respect to t in the simplex (see Appendix B). This is the compositional part of the closed system (3), where the vector $\mathbf{y}$ is a function of the x_i's. The compositional system (7) is not linear in the simplex. Also from appendix B, Theorem 2, the simplicial Equation (7) is the compositional part of the system (3) even in the case that the system is not closed. In this non-closed case, the differential equations (5) are not the equations describing the evolution of the compositional components; this only occurs whenever the total mass is constant.

In order to study the stability of the compositional system (7), it can be expressed in coordinates of the simplex $\mathcal{S}^D$. These coordinates are found using the isometric log-ratio transformation, ilr, (Appendix A),

$$\mathbf{u} = \mathrm{ilr}(\mathbf{x}) = (\log\mathbf{x})\Psi^t\ ,$$

where Ψ is the $(D-1, D)$ matrix whose rows are the clr-coefficients of the selected orthogonal basis of $\mathcal{S}^D$ (see Appendix A). Applying ilr-transformation in Equation (7) and using the properties of the derivative in the simplex

$$\frac{d}{dt}\mathbf{u} = \mathrm{ilr}(D^{\oplus}\mathbf{x}) = \mathbf{y}\Psi^t\ ,$$

where $\mathbf{y}$ still contain the ratios of x_i's as shown in (6). To obtain the expression of these ratios in terms of the coordinates, the inverse ilr-transformation (Appendix A) can be used to obtain

$$\mathbf{u} = \mathrm{clr}(\mathbf{x})\Psi^t \quad , \quad \mathbf{u}\Psi = \mathrm{clr}(\mathbf{x})\ ,$$

The desired ratios can be expressed as differences of the clr, using the column-vectors

$$\mathbf{v}(i,j) = \mathbf{e}_i - \mathbf{e}_j\ ,\ i, j = 1, 2, \ldots, D\ ,$$

where $\mathbf{e}_i$ is the i-th unitary vector of the canonical basis of $\mathbb{R}^D$. The ratios are now

$$\frac{x_i}{x_j} = \exp[(\mathbf{u}\Psi)\mathbf{v}(i,j)]\ ,\ i, j = 1, 2, \ldots, D\ .$$

Hence, i-th component of $\mathbf{y}$ is

$$y_i = \sum_{j=1}^{D}\alpha_j^i\exp[(\mathbf{u}\Psi)\mathbf{v}(j,i)]\ , \tag{8}$$

and Equation (7) is

$$\frac{d}{dt}\mathbf{u} = \left[\ldots, \sum_{j=1}^{D}\alpha_j^i\exp[(\mathbf{u}\Psi)\mathbf{v}(j,i)], \ldots\right]\Psi^t\ , \tag{9}$$

where only the i-th component has been specified. Once the solution of (9) is obtained using some quadrature method, the compositional solution is obtained using the inverse ilr transformation (see Appendix A)

$$\mathbf{x} = \mathcal{C} \exp(\mathbf{u}\Psi) \ .$$

This compositional solution can be easily obtained solving the linear system of masses (3) and then applying closure to the solution. Therefore, the equations in (9) are not useful to solve the system of EDO's but to study their qualitative behaviour.

3 Stability analysis

Stability analysis concern to critical points of the system (9). A point in the coordinate space $\mathbf{c}$ is a critical point if the right-hand-member of (9) vanishes for $\mathbf{u} = \mathbf{c}$. There are cases where there is no critical point for the system. Then, all possible solutions come from infinity and go to infinity and in all points of the coordinate space the solution is unique. From the compositional point of view, this means that, for all solutions, the proportion of some parts tend to vanish at infinite time. Alternatively, there are cases in which there is some critical point $\mathbf{c}$. Then, stability of a non-linear system of ODE's like (9) can be studied using its linearised form as stated in a well-known Liapunov theory. For simplicity, stability in the case $D = 3$ is detailed in the following results that can be found in many textbooks (Lefschetz, 1977; Plaat, 1974; Simmons, 1993).

Consider the system

$$\begin{aligned} \frac{du_1}{dt} &= \beta_1^1 u_1 + \beta_2^1 u_2 \ , \\ \frac{du_2}{dt} &= \beta_1^2 u_1 + \beta_2^2 u_2 \ , \end{aligned} \tag{10}$$

whose critical point is $u_1 = 0$, $u_2 = 0$. Its characteristic equation is

$$Q(m) = \begin{vmatrix} \beta_1^1 - m & \beta_2^1 \\ \beta_1^2 & \beta_2^2 - m \end{vmatrix} = m^2 - (\beta_1^1 + \beta_2^2)m + (\beta_1^1\beta_2^2 - \beta_2^1 + \beta_1^2) = 0$$

If m_1, m_2 are the roots of equation $Q(m) = 0$, then set $p = -(m_1 + m_2)$ and $q = m_1 m_2$. Stability of the system (10) can be described in terms of p, q as follows. If $p^2 - 4q < 0$ and $p \neq 0$, the critical point is a focus, that is unstable if $p < 0$ and asymptotically stable if $p > 0$; Figure 1 shows an example, with curves in coordinates (left) and the corresponding curves in the simplex $\mathcal{S}^3$ (right). If $p^2 - 4q < 0$ and $p = 0$, the critical point is a centre; Figure 2 shows an example in coordinates (left) and in the ternary diagram (right). If $p^2 - 4q > 0$ and $q > 0$, critical point is a node, unstable whenever $p < 0$ and asymptotically stable if $p > 0$; Figure 3 shows an example (coordinates, left; ternary diagram, right). Finally, if $p^2 - 4q > 0$ and $q < 0$, the critical point corresponds to a (unstable) saddle point (Fig. 4).

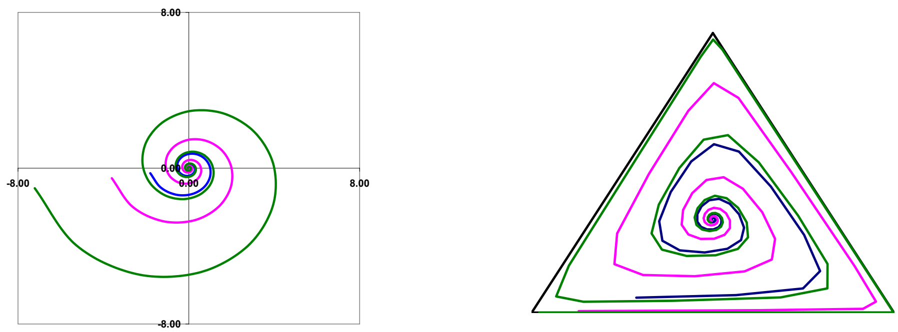

Figure 1. Orbits of a focus in coordinates (left) and in the ternary diagram (right)

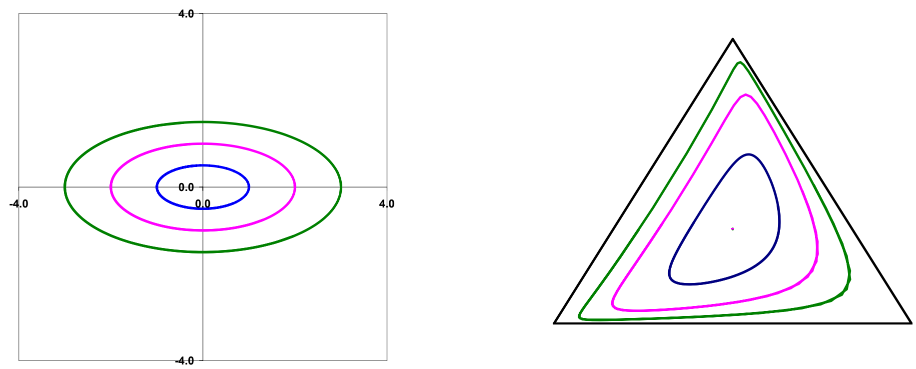

Figure 2. Orbits of a centre in coordinates (left) and in the ternary diagram (right)

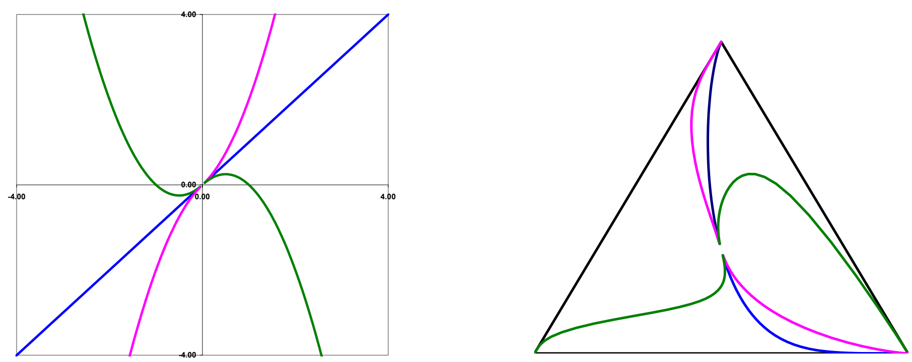

Figure 3. Orbits of a node in coordinates (left) and in the ternary diagram (right)

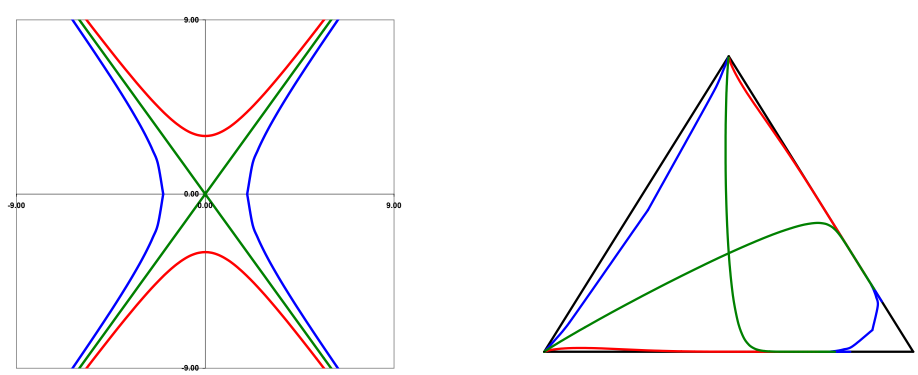

Figure 4. Orbits of a (unstable) saddle-point in coordinates (left) and in the ternary diagram (right)

4 Examples

The bismuth (Bi^{212}) radioactive decay has been selected to illustrate the study of stability. Following Moral and Pacheco (2003), the half-life of Bi^{212} is 60.55 min equivalent to a radioactive constant $\lambda_1 = \log 2/60.55 = 0.01145$. It disintegrates, via alpha emission, into Pb^{208}, which is a stable isotope, with frequency 64.06%. Alternatively, Bi^{212} decays (35.94%) into Tl^{208} , which again decays into Pb^{208} with half-life 3.053 min ($\lambda_2 = 0.22704$). Partial radioactive constants $\lambda_1' = (0.3594)(0.01145)$ and $\lambda_1'' = (0.6406)(0.01145)$ account for the rate in which Bi^{212} is transformed into Tl^{208} and Pb^{208} respectively. The system formed by these three nuclides: Bi^{212} (x_1), Tl^{208} (x_2) and Pb^{208} (x_3) constitute approximately a closed system (ignoring alpha emissions). The system can be represented as:

$$\begin{tikzcd}
x_1 : \mathrm{Bi}^{212} \arrow[rr] \arrow[dr] & & x_3 : \mathrm{Pb}^{208} \\
& x_2 : \mathrm{Tl}^{208} \arrow[ur] &
\end{tikzcd}$$

The mass equations of the system are

$$\frac{d}{dt}\begin{pmatrix} N_1 \\ N_2 \\ N_3 \end{pmatrix} = \begin{pmatrix} -\lambda_1 & 0 & 0 \\ \lambda_1' & -\lambda_2 & 0 \\ \lambda_1'' & \lambda_2 & 0 \end{pmatrix}\begin{pmatrix} N_1 \\ N_2 \\ N_3 \end{pmatrix} .$$

Figure 5 shows the evolution of the proportion of isotopes for initial conditions, $x_1(0) = 40$, $x_2(0) = 50$, $x_3(0) = 10$ in percent of mass.

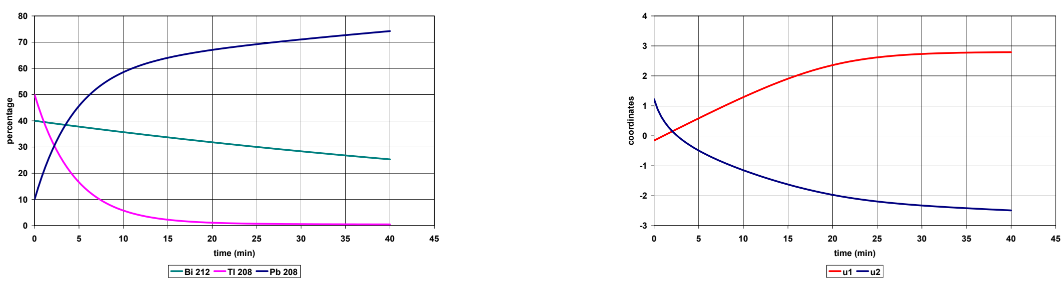

Figure 5. Evolution of the system Bi-Tl-PB in mass percentage (left) and in coordinates (right). Initial conditions are $x_1(0) = 40$, $x_2(0) = 50$, $x_3(0) = 10$

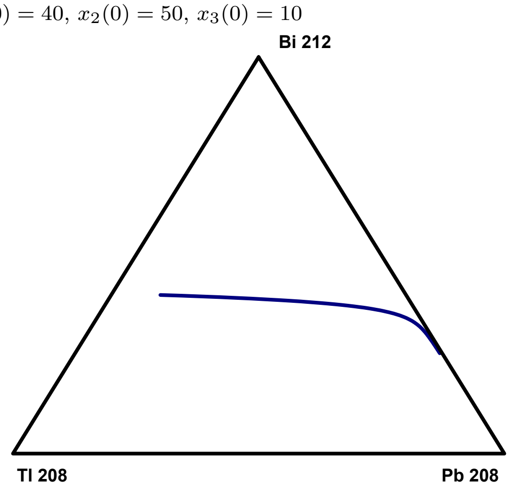

Figure 6. Orbit of the system Bi-Tl-PB in the ternary diagram. Initial conditions are $x_1(0) = 40$, $x_2(0) = 50$, $x_3(0) = 10$

The compositional system (9) is

$$
\begin{aligned}
\frac{du_1}{dt} &= -\frac{\lambda_1'}{\sqrt{2}} \exp\left(\sqrt{2}u_1\right) + \frac{\lambda_2 - \lambda_1}{\sqrt{2}} \\
\frac{du_2}{dt} &= \frac{\lambda_1'}{\sqrt{6}} \exp\left(\sqrt{2}u_1\right) - \frac{2\lambda_1''}{\sqrt{6}} \exp\left(\frac{u_1}{\sqrt{2}} + \frac{\sqrt{3}u_2}{\sqrt{2}}\right) \\
&\quad -\frac{2\lambda_2}{\sqrt{6}} \exp\left(-\frac{u_1}{\sqrt{2}} + \frac{\sqrt{3}u_2}{\sqrt{2}}\right) - \frac{\lambda_1 + \lambda_2}{\sqrt{6}}
\end{aligned}
$$

where the matrix Ψ has been chosen

$$
\Psi = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \end{pmatrix} . \tag{11}
$$

The main characteristics of (11) is that it is non-linear and it has no-critical points. Figure 5 and 6 show the behaviour of the solution of the non linear system of equations (7), where coordinates go to infinity (Fig. 5, right). with the time and Pb^{208} cumulates the total mass of the system.

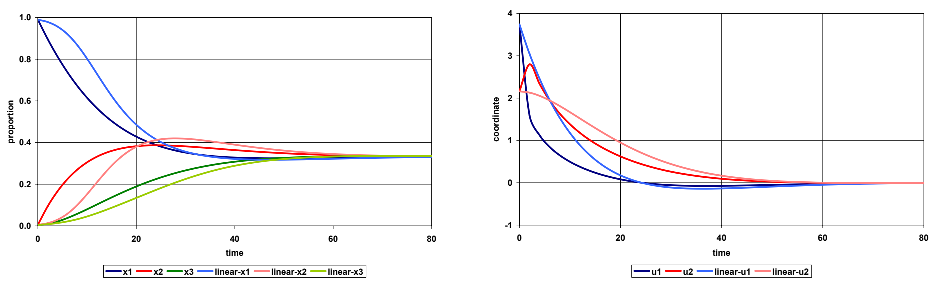

Figure 7. Evolution of the cycle system in mass percentage (left) and in coordinates (right). Full compositional system, intens colours; linearised system, pale colours. Initial conditions are $x_1(0) = 0.99$, $x_2(0) = 0.005$, $x_3(0) = 0.005$

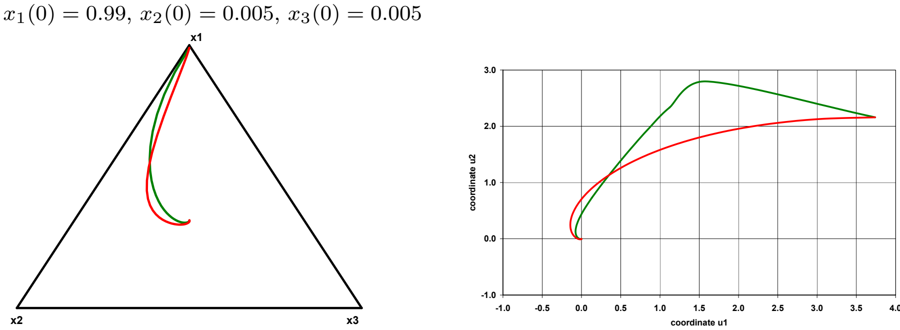

Figure 8. Orbit of the cyclic system in the ternary diagram (left) and in the coordinate plane (right). Green: full compositional system; red: linearized system. Initial conditions are $x_1(0) = 0.99$, $x_2(0) = 0.005$, $x_3(0) = 0.005$

A second example shows that simple systems may have critical points. Consider some elements which can be in three different states, namely 1, 2, 3. Assume that elements in a given state have independent exponential life. When the failure occurs the state changes to the next state cyclically. Assume that the half-life in each state is 13.9 time units corresponding to a decay constant $\lambda = \log 2/13.9 = 0.05$. The proportions of elements in each class are denoted x_1, x_2 and x_3. This corresponds to the cyclic scheme

$$
\begin{array}{ccc}
x_1 & \longleftarrow & x_3 \\
 & \searrow \quad \nearrow & \\
 & x_2 &
\end{array}
$$

The compositional system is

$$
\frac{d}{dt}(x_1, x_2, x_3) = (x_1, x_2, x_3) \begin{pmatrix} -\lambda & \lambda & 0 \\ 0 & -\lambda & \lambda \\ \lambda & 0 & -\lambda \end{pmatrix} .
$$

This system, expressed using coordinates associated with the basis corresponding to Ψ in (11), is the non-linear system

$$
\begin{aligned}
\frac{du_1}{dt} &= \frac{\lambda}{\sqrt{2}} \exp\left(-\frac{u_1}{\sqrt{2}} - \frac{3u_2}{\sqrt{6}}\right) - \frac{\lambda}{\sqrt{2}} \exp(\sqrt{2}u_1) \ , \\
\frac{du_2}{dt} &= \frac{\lambda}{\sqrt{6}} \exp\left(-\frac{u_1}{\sqrt{2}} - \frac{3u_2}{\sqrt{6}}\right) - \frac{\lambda}{\sqrt{6}} \exp(\sqrt{2}u_1) - \frac{2\lambda}{\sqrt{6}} \exp\left(-\frac{u_1}{\sqrt{2}} + \frac{3u_2}{\sqrt{6}}\right) .
\end{aligned} \tag{12}
$$

For initial conditions $x_1(0) = 0.99$, $x_2(0) = 0.005$, $x_3(0) = 0.005$, the compositional evolution is shown in Figure 7 (left, intense colours). The system (12) has a critical point in $u_1 = 0$, $u_2 = 0$. After linearisation, the system in coordinates is

$$
\begin{aligned}
\frac{du_1}{dt} &= -\frac{3\lambda}{2}u_1 - \frac{\sqrt{3}\lambda}{2}u_2 \ , \\
\frac{du_2}{dt} &= \frac{\sqrt{3}\lambda}{2}u_1 - \frac{3}{2}u_2 \ .
\end{aligned} \tag{13}
$$

The solution is shown in Figure 7 (right, pale colours) and the corresponding evolution of the composition in Figure 7 (left, pale colours). Stability of the critical point is studied using the linear system (13). It is identified as a stable focus as confirmed by the behaviour of the solution shown in Figure 7. The solution in the phase plane of coordinates is shown in Figure 8 in coordinates (right) and in the ternary diagram (right). Also the solutions of the non-linear system are compared to the linearised system ones. The stable behaviour is clearly shown and the solution tend to the barycentre of the ternary diagram when time increase. For a stable focus trajectories go to the critical point following a spiral-shaped curve. This behaviour occurs for any initial conditions.

Conclusion

Systems of differential equations modelling the evolution of the mass of different species can be decomposed into two parts: that controlling the evolution of mass; and the compositional part describing the change of the proportion of the different masses. The compositional part is properly treated in the framework of the Aitchison geometry of the simplex and using the corresponding derivatives.

The study of the compositional part of a system is necessary because the character of the mass system and the compositional part of it may have different characteristics (linear or non-linear; stable and unstable). Attention has been centred on closed mass linear systems for which the mass evolution is just constant. The compositional part is non-linear in the framework of the simplicial geometry. In order to study the stability, this non-linear system has been linearised if there is some critical point. No critical point appears in the 3 species case and illustrated with the disintegration of the Bi^{212} into Tl^{208} and Pb^{208}. The compositional evolution is non-linear and the stability corresponds to an asymptotically stable node. Alternatively, a cyclic change example shows a critical point identified as a stable focus.

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Appendix A. Orthogonal coordinates in the simplex

A brief description of the Aichison geometry of the simplex follows. More details can be found in Aitchison et al. (2002); Pawlowsky-Glahn and Egozcue (2001); Egozcue et al. (2003); Egozcue and Pawlowsky-Glahn (2005, 2006) Let $\mathcal{S}^D$ be the simplex of D parts defined as

$$\mathcal{S}^D = \left\{ \mathbf{x} = [x_1, x_2, \ldots, x_D] \middle| x_i > 0 \ , \ \sum_{i=1}^{D} x_i = \kappa > 0 \right\} \ ,$$

where $[\cdot]$ stands for row-vectors. The simplex $\mathcal{S}^D$ can be structured as an Euclidean space (Billheimer et al., 2001; Pawlowsky-Glahn and Egozcue, 2001) considering the operations perturbation, $\oplus$, and powering, $\odot$, defined as

$$\mathbf{x} \oplus \mathbf{y} = \mathcal{C}[x_1 y_1, x_2 y_2, \ldots, x_D y_D] \ , \ \alpha \odot \mathbf{x} = \mathcal{C}[x_1^\alpha, x_2^\alpha, \ldots, x_D^\alpha] \ ,$$

where $\mathcal{C}$ denotes closure of the vector to κ (here assumed the unit 1); and $\mathbf{x}$, $\mathbf{y} \in \mathcal{S}^D$, and $\alpha \in \mathbb{R}$. With these operations $\mathcal{S}^D$ is a vector space of dimension $(D-1)$. Moreover, the inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_a = \sum_{i=1}^{D} \log x_i \cdot \log y_i - \frac{1}{D} \left(\sum_{j=1}^{D} \log x_j \right) \left(\sum_{k=1}^{D} \log y_k \right) \ ,$$

is compatible with the perturbation and gives the metric structure of the Euclidean space. The subscript $(\cdot)_a$ is referred to J. Aitchison who introduced the main elements of the geometry of the simplex (Aitchison, 1986). The norm and the distance are defined accordingly:

$$\|\mathbf{x}\|_a = (\langle \mathbf{x}, \mathbf{x} \rangle_a)^{1/2} \quad , \quad d_a(\mathbf{x}, \mathbf{y}) = \| \langle \mathbf{x} \ominus \mathbf{y} \rangle_a \|_a^{1/2} \ ,$$

where $\ominus$ is the opposite of perturbation, i.e. $\ominus \mathbf{x} = \oplus((-1) \odot \mathbf{x})$.

The centred log-ratio transformation, clr : $\mathcal{S}^D \to \mathbb{R}^D$, is and isometry of the simplex on the subspace of dimension $(D-1)$ of $\mathbb{R}^D$. It is defined as

$$\mathrm{clr}(\mathbf{x}) = [\xi_1, \xi_2, \ldots, \xi_D] \ , \ \xi_i = \log \frac{x_i}{g(\mathbf{x})} \ ,$$

where $g(\cdot)$ denotes the geometric mean of the components in the argument. The components of $\mathrm{clr}(\mathbf{x})$ add to zero, and this is the equation of the mentioned subspace of $\mathbb{R}^D$. The inverse transformation is

$$\mathrm{clr}^{-1}(\boldsymbol{\xi}) = \mathcal{C} \exp(\boldsymbol{\xi}) \ .$$

Orthonormal bases in $\mathcal{S}^D$ are constituted by $D-1$ compositions. Consider one of such bases with vectors, $i = 1, 2, \ldots, D-1$,

$$\mathbf{e}_i = \mathcal{C} \exp(\boldsymbol{\psi}_i) \ , \ \mathrm{clr}(\mathbf{e}_i) = \boldsymbol{\psi}_i \ , \ \langle \boldsymbol{\psi}_i, \boldsymbol{\psi}_j \rangle_a = \delta_{ij} \ .$$

The function that assigns the coordinates in this basis to a composition is called isometric log-ratio transformation, ilr : $\mathcal{S}^D \to \mathbb{R}^{D-1}$ and has the expression

$$\mathbf{x}^* = \mathrm{ilr}(\mathbf{x}) = [\langle \mathbf{x}, \mathbf{e}_1 \rangle_a, \langle \mathbf{x}, \mathbf{e}_2 \rangle_a, \ldots, \langle \mathbf{x}, \mathbf{e}_{D-1} \rangle_a] = \mathrm{clr}(\mathbf{x}) \cdot \Psi^t \ ,$$

where the matrix $\Psi = (\mathrm{clr}(\boldsymbol{\psi}_1)^t, \mathrm{clr}(\boldsymbol{\psi}_1)^t, \ldots, \mathrm{clr}(\boldsymbol{\psi}_D)^t)^t$, i.e. is a $(D-1, D)$-matrix whose rows are $\mathrm{clr}(\mathbf{e}_i)$. The inverse of ilr is obtained as

$$\mathbf{x} = \mathrm{ilr}^{-1}(\mathbf{x}^*) = \bigoplus_{i=1}^{D-1} (x_i^* \odot \mathbf{e}_i) = \mathcal{C} \exp(\mathbf{x} \Psi^t) \ .$$

The rows of the matrix Ψ add to zero, the row-wise sum of squares of the entries is 1 and the rows, as real vectors, are orthogonal. The matrix satisfy $\Psi^t \Psi = I_D - D^{-1} \mathbf{1}_D^t \mathbf{1}_D$ and $\Psi \Psi^t = I_D$.

Appendix B. Derivatives in the simplex

The definition of derivative in the simplex (Aitchison et al., 2002; Barceló-Vidal and Martín-Fernández, 2002; Aitchison and Egozcue, 2005) and the main result on its expression is presented. Consider a function $\mathbf{f} : \mathbb{R} \to \mathcal{S}^D$, that may be interpreted, e.g., as an evolution of a composition with time. The way of describe change of a function with respect to a parameter is the ordinary derivative. However, when the images of the function are not real, the scale is no longer related to the Lebesgue measure, and the difference is not substraction, an alternative definition is required.

Definition. 1 (Derivative)**.** *If the limit*

$$D^{\oplus}\mathbf{f}(t) = \lim_{h\to 0} \frac{1}{h} \odot (\mathbf{f}(t+h) \ominus \mathbf{f}(t)) \ , \tag{14}$$

exists, then $\mathbf{f}$ *is differentiable at* t *and* $D^{\oplus}\mathbf{f}(t)$ *is the derivative of* $\mathbf{f}$ *at* t.

Theorem. 1. *If* $\mathbf{f}$ *is differentiable at* t*, then*

$$\begin{aligned} D^{\oplus}\mathbf{f}(t) &= \mathrm{clr}^{-1}\left(\frac{d}{dt}\mathrm{clr}(\mathbf{f}(t))\right) \\ &= \mathrm{ilr}^{-1}\left(\frac{d}{dt}\mathrm{ilr}(\mathbf{f}(t))\right) \\ &= \mathcal{C}\exp\left(\frac{d}{dt}\log(\mathbf{f}(t))\right) \ , \end{aligned}$$

where d/dt *denotes ordinary derivative of a real function.*

Proof. The term following the limit in Eq.(14) can be written using clr and ilr and their isometric character,

$$h^{-1} \odot (\mathbf{f}(t+h) \ominus \mathbf{f}(t)) = \mathrm{clr}^{-1}\left[h^{-1} \cdot (\mathrm{clr}(\mathbf{f}(t+h)) - \mathrm{clr}(\mathbf{f}(t)))\right]$$

$$= \mathcal{C}\exp\left[h^{-1} \cdot (\log(\mathbf{f}(t+h)) - \log(\mathbf{f}(t)) - (\log g(\mathbf{x}(t+h) - \log g(\mathbf{x}(t)))))\right]$$

$$= \mathrm{ilr}^{-1}\left[h^{-1} \cdot (\mathrm{ilr}(\mathbf{f}(t+h)) - \mathrm{ilr}(\mathbf{f}(t)))\right] \ .$$

The limit can be taken inside the arguments of clr^{-1}, ilr^{-1}, exp, because they are continuous functions. The term with the difference of two logarithms of geometric means cancel out in the limit due to necessary continuity of $\mathbf{x}$ to be derivable. The expression of the derivatives is obtained taking the limits and identifying the corresponding incremental ratios. □

An important result is that compositional derivative conmutes with closure, i.e. compositional derivative can be applied to non-closed real positive vectors.

Theorem. 2. *Let* $\mathbf{N} : \mathbf{R} \to \mathbb{R}_+^{\mathbf{D}}$ *be a positive real vector valued function denoted* $\mathbf{N}(t) = (N_1(t), \ldots, N_D(t))$*. Define* $N(t)$ *as a positive real function of the components* $N_i(t)$*, e.g.* $N(t) = \sum_{i=1}^{D} N_i(t)$*. If* $dN(t)/dt$ *and* $dN_i(t)/dt$*,* $i = 1, 2, \ldots, D$ *exist at* t*, then*

$$D^{\oplus}\left((N(t))^{-1}\mathbf{N}(t)\right) = D^{\oplus}\mathbf{N}(t) \ ,$$

or equivalently

$$D^{\oplus}\mathcal{C}\mathbf{N} = \mathcal{C}D^{\oplus}\mathbf{N} = D^{\oplus}\mathbf{N} \ .$$

Proof. Using Theorem 1,

$$D^{\oplus}\left((N(t))^{-1}\mathbf{N}(t)\right) = \mathcal{C}\exp\left[\frac{d}{dt}\log(N(t))^{-1}\mathbf{N}(t)\right] = \mathcal{C}\left\{\exp\left[\frac{d}{dt}\log\mathbf{N}\right] \cdot \exp\left[\frac{d}{dt}\log N \cdot \mathbf{1}_D\right]\right\} \ ,$$

Since the second exponential term is equal in each component, it cancels with the closure, and the result is $D^{\oplus}\mathbf{N}$. □