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Calculus on the Simplex**

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In practice, evolution of compositions in time, space, temperature, etc. appear very frequently. These situations can be described using functions defined on a real variable with values in the simplex $\mathcal{S}^D$. Changes of a chemical composition, changes of vote intention, evolution of employment in time are examples. Modeling these compositional changes requires the study of these simplex-valued functions and elementary concepts like derivative, describing the rate of change, or integral, to give mean values or summary descriptors. According to the Euclidean geometry defined on the simplex, we introduce in the first part of this communication the definitions and properties of limit, continuity, ordinary derivative and integral of a simplex-valued function with real domain, following the classical lines of real analysis. Images of the considered functions are represented in several forms: elements of the simplex, real vectors with positive components, real vectors of coordinates with respect to a given basis. All these representations are necessary for a proper interpretation of the results. Although the development is parallel to standard calculus of vector-functions, this variety of representations make some expressions peculiar, and require re-definitions of elementary concepts like simplicial derivatives or integrals.

In other studies the analyst assumes that the response variable y depends on the proportions $x_1, \ldots, x_D$ of D ingredients or components present in a specific mixture and not on its total amount. These proportions are often expressed by volume, by weight, by mole fraction, etc. In mathematical terms, the response variable y is a real or vector-valued function φ whose domain is a subset of the simplex space. In many practical situations, the expression $y = \varphi(x_1, \ldots, x_D)$ is unknown and the emphasis is on fitting the simplest model to the experimental data. In other scenarios, the function φ can be deduced from physical laws or from other sources. In such cases, the standard interpretation of function φ from differential calculus is not directly applicable because of the constraint $x_1 + \ldots + x_D = 1$ of its components. For example, the partial derivative $(\partial\varphi/\partial x_i)(\mathbf{x})$ of φ at $\mathbf{x}$ with respect to x_i cannot be interpreted as the variation of the function φ with respect to the change in x_i when the other components are held constant because any change in x_i requires changing at least one of the other components. In the second part of this communication we develop the main topics of compositional differential calculus of vector-valued functions without delving into mathematical aspects related to the problems of existence and uniqueness. We explain how the introduction of the new concept of *compositional derivative* of a function defined on the simplex, together with the use of simplicial operators, allows us to handle the differential calculus of these functions by analogy to standard differential calculus.

The topics of differential calculus introduced here are an adaptation of classical concepts that can be found in any standard textbook on multivariate differential calculus. This communication is the summary of the contents of the two papers Egozcue

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et al. (2011) and Barceló et al. (2011) forthcoming in *Elements of Simplicial Linear Algebra and Geometry*, John Wiley & Sons, Ltd.

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Referencias

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