Electronic tongues, electronic languages and machine learning for materials science

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The ongoing revolution with artificial intelligence applications in the Internet of Things and various computational systems is likely to change the landscape of science and technology in the next few decades. The pace of change is such that one may envisage for the first time in history the possibility of machine-generated knowledge with no human intervention. This could result from the convergence of two relatively separate movements. The first is broadly known as Big Data through which large amounts of data are mined and processed to generate knowledge. Machine learning is central for transforming information into knowledge. The second movement is associated with natural language processing, where researchers and developers attempt to make machines (computational systems) capable of communicating in natural languages (Portuguese, English, Chinese, etc) as an ultimate goal. Again, these systems are trained with massive amounts of data, as is the case of current machine translation systems, with machine learning also being crucial. Before such ambitious endeavors can become a reality, much has to be done in various areas. For example, the data from which the machines will be trained to learn have to be generated and stored, which is normally performed with a variety of devices. Indeed, sensing and biosensing will be ubiquitous for applications in the Internet of Things.

In this presentation an overall discussion will be given of the requirements for the convergence of the aforementioned movements, with particular emphasis on the importance of materials science in general, and polymers in particular. Electronic tongues (e-tongues) were chosen as paradigmatic systems where this convergence can take place. An e-tongue comprises an array of sensing units whose electrical responses upon analyzing a liquid sample can be combined to establish a “fingerprint” of said liquid.[1] Applications of e-tongues go beyond the classification of beverages and monitoring of water quality, for they can be extended to liquids not meant for human consumption.

The sensing units of an e-tongue are made of ultrathin films that may contain nanomaterials, polymers and even biomolecules for the cases in which some degree of specificity in the interactions with the analyte is desired. The latter has been exploited in e-tongues functioning as biosensors for distinguishing between similar diseases with no false positives.[2] Recent advances in e-tongues related to polymers and materials science have arisen from the use of microfluidic devices in distinct ways. While preserving the positive feature of a variety of possible materials to be employed in the sensing units, the microfluidic e-tongues provide a faster response and are amenable to miniaturization. This is especially relevant for widespread dissemination of e-tongues, as in point-of-care diagnostics. A single-response e-tongue made with microwires, for instance, may solve the problem of multiple calibrations when sensing units have to be replaced.[3]

The data generated by an individual e-tongue is already considerable to justify the use of statistical and computational methods to classify the samples. There is ample literature in classification methods, which may include information visualization techniques, in addition to supervised and non-supervised machine learning algorithms. Machine learning, for instance, has been applied to correlate the data from an e-tongue made of conducting polymers with the human perception of taste for coffee samples.[4]

The connection between e-tongues and e-languages can be established in two ways. On one hand, classification methods for treating the e-tongue data are in many cases the same used in text analytics. In fact, one of the most successful multidimensional projection techniques for classifying samples with sensors and biosensors was conceived to classify texts. On the other hand, classifying text and even employing e-languages may be crucial for the success of various smart systems, in the Internet of Things and in computer-assisted diagnosis. Indeed, the stringent requirements to build a computer-assisted diagnosis system include integration of data of different natures and formats[5]. E-tongues and e-languages will be merged seamlessly in this type of integrated application.

Finally, in addition to discussing these recent developments and the trends for the next few years in machine learning and materials science for e-tongues and similar applications, the impact of such progress will be evaluated. Emphasis will be given to the effects on the job market and on the ways education will have to be adapted to cope with such rapid changes.

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