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Visual signal perception in two-dimensional elemental mapping –toward new criteria for instrumental detection limits

In analytical chemistry, an essential figure of merit for assessing the performance of chemical measurements is the Limit of Detection (LOD), which represents the lowest concentration of a chemical substance in a measured sample that can be estimated with a reasonably high level of confidence. According to a well-established formula by IUPAC, LOD is calculated as the mean plus 3.3 times the standard deviation of the blank measurement, where blank is ideally a sample devoid of the substance of interest. This definition has been widely accepted in calibration approaches and instrumental methods with one-dimensional (1D) data settings such as chromatographic, electrochemical and spectroscopic methods. However, in two-dimensional (2D) data from elemental imaging and mapping techniques, signals below the LOD often remain visually discernible. This discrepancy can be attributed to two unique capabilities of visual perception –a nonlinear sensitivity to subtle intensity changes of perceived objects, and the propensity to integrate spatially redundant information into salient features. Inspired by developments in psychophysics and perceptual image coding, we propose the so-called Just-Noticeable Difference (JND) as an alternative metric for chemical data analysis in 2D contexts. The JND refers to the smallest difference between two stimuli that human senses can still register. By utilizing the JND as a guiding principle in targeting low-contrast signals, we provide a novel framework for improving the interpretation of detection limits in 2D data and recognition of subtle signals that might not meet traditional LOD criteria but are nonetheless discernible due to their spatial context. The potential of JND as a signal detection criterion, presented as a proof of concept on mapping data of two cutting-edge instrumental analytical methods, laser ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) and laser-induced breakdown spectroscopy (LIBS), is compared to the standard LOD metric. Theoretical investigations of elemental maps from an artificially constructed sample with known composition allude to the possibility for more accurate assessments of elemental concentrations and a better leverage of spatial information inherent in images. A general scheme for image processing and assessment in terms of the two metrics is developed, which is suitable for a wide variety of applications from biology to physical sciences.

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