Decremental Active Learning for Optimized Self-Adaptive Calibration in Viscose Production

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In viscose production, it is important to monitor the concentration of several substances (H2SO4, Na2SO4 and ZnSO4) as part of the spin bath in order to assure a high quality of the final product. The acid and the two salts govern the precipitation and agglomeration of the cellulose from viscose solution and the formation of the viscose fibre. During on-line production, these process parameters usually show a quite high dynamics depending on the fibre type that is produced and on environmental influences. In such cases, conventional chemometric models, such as principal components regression, partial least squares regression, locally weighted regression and others [1][2], as well as non-linear techniques recently employed in calibration, e.g. [3][4], may show severe downtrends in performance when quantifying the concentrations of new on-line data. This is because they are established once based on pre-collected calibration spectra and kept fixed during the whole life-time of the on-line process, thus not being able to adapt to dynamically changing situations at the system. Recently, a new concept termed as eChemo (evolving chemometric models), was introduced in [5] to overcome these deficiencies of static calibration. It possesses the ability to self-adapt and re-calibrate based on newly recorded on-line spectra obtained through FT-NIR measurements, but it requires permanent supervision, i.e. real values measured by means of a titration automaton, which are time intensive and expensive from an industrial viewpoint.

We propose an alternative approach, based on self-adaptive calibration models within a sliding window concept, which introduces more flexibility in the incremental learning phase and especially also in the forgetting process of older samples. It consists of a window of W samples that is updated every R incoming new samples by means of substitution of one sample by the new one. The selection of the outgoing sample is guided by a two-stage selection process (termed as decremental active learning): i) we substitute one sample in the current window by the new sample, if they are significantly similar in terms of a spectral similarity measure based on Bayesian statistics [6]. ii) If we substitute no sample in the first stage, W models are created leaving a different sample out in each of them, thus we choose the sample which is out of the best model as the less informative one. This approach permits introducing more flexibility in terms of self-adjusting learning parameters and self-optimizing input dimensionality for the calibration models, thus allowing the integration of an input structure change, which is not possible in eChemo. Moreover, it also achieves accurate results and requires much (about 45-60 times) less real values, leading to a huge computational time and financial saving. We show that our approach significantly outperforms conventional S-o-A models, eChemo, and other decremental strategies, when using real world data streams.

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