

Adaptive Polynomial Approximation of Chromatographic Peaks

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Savitsky-Golay algorithm is one of the most frequently used noise filtration algorithms in chromatography. It is based on polynomial approximation of the chromatogram and provides excellent reduction of noise without big modification of peak shape. Besides, in some case it is difficult to implement it, as in the case of e.g. triangular peaks, like in capillary electrophoresis, optimal numbers of points for effective noise reduction for left and right slopes of the peak are significantly different.

We implemented peak approximation using different number of points for either slope of the peak, depending on the slope "width". This approximation allows accurate calculation of peak parameters even for very asymmetric peaks. This kind of peak approximation is complemented by effective noise filtration, also based on Savitsky-Golay algorithm.

As computers nowadays are much more powerful than before, for noise filtration we combined polynomial approximation with prediction of the confidence interval for all points of the approximated region. Chromatogram is approximated many times by the windows with one data point shift, and only points with better confidence interval are stored in the filtered chromatogram on every step. Results of this procedure coincide with original Savitsky-Golay approximation for smooth regions and give different prediction near sharp edges, disturbing chromatogram in a lesser extent. This procedure is especially useful for baseline noise filtration prior to peak detection.

Filtration and approximation results are compared using several examples from different kinds of chromatography.

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