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Gradient design for liquid chromatography using multi-scale optimization

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Highlights

- Optimal multi-linear gradients are designed using a multi-scale approach
- Gradients are outlined as a polygonal simplification from cubic splines
- Subdivision schemes allow the best accommodation to the local needs of each solute
- Long analysis times and excessive steeped slopes close to the peaks are penalized
- Variable weight for critical peaks and excessive weight for unresolved peaks are considered

Abstract

In reversed phase-liquid chromatography, the usual solution to the "general elution problem" is the application of gradient elution with programmed changes of organic solvent (or other properties). A correct quantification of chromatographic peaks in liquid chromatography requires well resolved signals in a proper analysis time. When the complexity of the sample is high, the gradient program should be accommodated to the local resolution needs of each analyte. This makes the optimization of such situations rather troublesome, since enhancing the resolution for a given analyte may imply a collateral worsening of the resolution of other analytes. The aim of this work is to design multi-linear gradients that maximize the resolution, while fulfilling some restrictions: all peaks should be eluted before a given maximal time, the gradient should be flat or increasing, and sudden changes close to eluting peaks are penalized. Consequently, an