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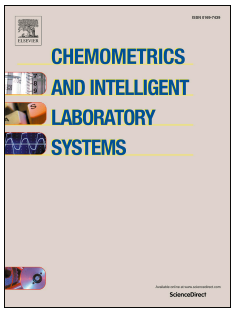

Time fractional super-diffusion model and its application in peak-preserving smoothing

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Time Fractional Super-Diffusion Model and Its Application in Peak-Preserving Smoothing

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Abstract: The super-diffusion model is suggested for peak-preserving smoothing. In this model, the time derivative on the left of the classical diffusion model is replaced with the time fractional derivative. Because of the weight property of the fractional derivative, the super-diffusion model can further improve the smooth performance of the classical nonlinear diffusion model. An explicit difference scheme and an implicit difference scheme are given. Then some comparisons between the proposed model and the classical nonlinear diffusion model are done. The results indicate the proposed model outperforms the classic nonlinear diffusion model. In the end, the proposed method is used to smooth a nuclear magnetic resonance spectroscopy and a mass spectrometry.

Key words: Diffusion filtering; fractional diffusion; smoothing; mass spectrometry; regularization method

1. Introduction

Derivative spectroscopy has widely applied in analytical science. However, experimental spectra usually are a mixture of noise and signal. Therefore, it is necessary to reduce the noise in the spectra and preserve the peak as much as possible. At present, The Savitzky–Golay method [1] is a widely used method, which is a generalization of the sliding average method. As an improved alternative to the Savitzky-Golay