Stochastic Regression Modeling of Noisy Spectra

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Deploying mass spectrometers in harsh environments often means compromising signal to noise ratio for the benefit of small size, ruggedness, low energy consumption and other technical considerations. Poor signal to noise presents the operator with the difficult proposition of having to determine the existence, position, and intensity of any and all peaks in the mass spectrum. Here we present a method to model mass spectra using stochastic differential equations (SDE) where both the drift (signal) and diffusion (noise) coefficients depend on time. The benefit of the SDE model is that it seeks to decompose the spectrum into signal plus noise. SDE modeling could yield enhanced peak picking information, a method to eliminate (or filter) peaks that have the same characteristic of approximated noise, and a simulation tool to generate large amounts of meaningful spectra in very little time.