DETERMINING THE EFFECTS OF NOISE IN EXPONENTIAL DATA

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In solid state NMR relaxation studies, the nuclei of the hydrogen atoms in the molecules under study are magnetically perturbed and their return to equilibrium is observed. Mathematical models fitted to nuclear relaxation data are exponential only in some cases. Additionally, measurements taken during experiments involving low NMR frequencies are often noisy. Noise can disguise the mathematical model of a data set. Therefore, it is sometimes difficult to determine which model, exponential or non-exponential, is appropriate for a set of data.

The degree to which data fits an exponential model can be determined by fitting the data to a stretched exponential function. A stretched exponential function, e^{x^β}, becomes an exponential function when β equals one. The degree to which a data set is exponential can be determined by fitting a stretched exponential to the data and observing the departure of β from one. However, this method does not differentiate between data sets that are truly non-exponential and data sets which are non-exponential due to noise in the data.

A computer code that simulates noisy NMR relaxation data can be used to study the effects of noise in exponential data by fitting data to a stretched exponential via simplex fitting routines. The simulation generates a series of equally spaced data points from the function $y(t) = (150e^{-Rt}) - 100$, where R is the relaxation rate and t is time, to simulate a single data set. A random number generator produces randomized noise, which is then added to the value of $y(t)$. The noisy data is fitted to both the previously mentioned exponential function and the following stretched exponential function $y(t) = (150e^{-(R^*t)^\beta}) - 100$, where R^* is also a relaxation rate for a stretched exponential. The code records the values and repeats the process, collecting additional values of R and β each run. After many runs, the code bins and plots the values of R and β as a histogram.