

The Laplace transform of a function $f(t)$ is defined as

$$\mathcal{L}\{f\}(s) = \int_0^\infty f(t)e^{-st} dt$$

where, in general, the transformed function denoted as $\bar{f}(s)$ is a complex-valued function of the complex variable s . In an NMR T_2 relaxation experiment, the signal intensity of a signal with time constant T_2 decays as $I_0(t)e^{-t/T_2}$. In a sample with multiple peaks, each with its own relaxation behaviour, the total integrated signal decays as

$$I(t) = \sum_n I_{0n} e^{-t/T_{2n}}$$

sampled at discrete time points $\{t_m\}$. This resembles a discrete version of the Laplace transform with $T_2 = 1/s$, where both the original and transformed functions are real-valued functions of real variables. The amplitudes of the relaxation components that exist in the signal, $\{I_{0n}\}$, can be extracted by inverting the Laplace transform.

Unlike the Fourier transform, however, the Laplace transform is not unitary and the inverse cannot be easily calculated¹. Writing the expression above in matrix form with the following redefinitions

$$\begin{aligned} \mathbf{b} &= [I(t_0) \ I(t_1) \ \dots \ I(t_m)]^\top \\ \mathbf{x} &= [I_{01} \ I_{02} \ \dots \ I_{0n}]^\top \\ \mathbf{A} &= \begin{bmatrix} e^{-t_1 s_1} & \dots & e^{-t_1 s_n} \\ \vdots & \ddots & \vdots \\ e^{-t_m s_1} & \dots & e^{-t_m s_n} \end{bmatrix} \end{aligned}$$

we have a system of linear equations

$$\mathbf{Ax} - \mathbf{b} = 0$$

which can be solved as an optimisation problem with constraints $x_i \geq 0$. The same approach can be used for T_1 recovery experiments by changing the functional form of the elements of the transformation matrix \mathbf{A} to recovery curves.

¹Numerical algorithms to compute the inverse exist (<https://link.springer.com/article/10.1007/s11075-012-9625-3>), but generally require the function to be sampled at a large number of arbitrary points, which is not compatible with experimentally acquired datasets.