

Brief Explanation of 1D NMR T2 Inversion with Tikhonov Regularization

The process of T2 inversion in NMR aims to extract a distribution of transverse relaxation times (T2) from multi-exponential decay data. Since this is an ill-posed problem, small errors in data can lead to large variations in the solution. Tikhonov regularization helps stabilize the inversion by imposing smoothness constraints.

Steps of Inversion

1. Data Acquisition:

- The measured signal $S(t)$ follows:

$$S(t) = \sum A_i \exp(-t / T_{2i}) + \text{noise}$$

- Here, A_i are the amplitudes, and T_{2i} are the transverse relaxation times.

2. Kernel Construction:

- A model matrix (kernel) is built based on possible T2 values:

$$K_{ij} = \exp(-t_j / T_{2i})$$

- This matrix transforms the T2 distribution into the measured decay signal.

3. Tikhonov Regularization:

- Instead of solving $KA = S$ directly (which can be unstable), we solve a regularized least-squares problem:

$$\min_A \|KA - S\|^2 + \lambda \|LA\|^2$$

- λ (regularization parameter) controls smoothness:

- Small $\lambda \rightarrow$ solution close to raw inversion (more noise).

- Large $\lambda \rightarrow$ over-smoothed solution.

- L is usually the identity matrix or a finite difference matrix enforcing smoothness.

4. Solving the Regularized System:

- Using methods like scipy's `lsq_linear`, we solve for A , ensuring non-negative solutions.

5. Visualization:

- The final T2 distribution ($A(T2)$) is plotted against T2, showing the relative abundance of each relaxation component.

Advantages of Tikhonov Regularization:

- Prevents overfitting to noise in experimental data.
- Provides a smoother, more interpretable T2 distribution.
- Ensures stability in ill-posed inversion problems.