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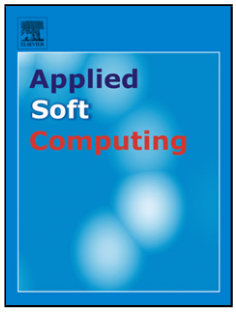

Title: Gaussian process regression for automated signal tracking in step-wise perturbed Nuclear Magnetic Resonance spectra

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Highlights

- Novel tracking method of signals in NMR spectra
- Modelling trajectories with Gaussian Process Regression model
- First time supervised machine learning model used for this tracking problem
- Method handles complex data problems: missing signals, noise and crossing trajectories
- Results of exeperiments show the benefits of proposed solution comparing to the reference distace-based approach.

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