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Smart sampling in time-domain spectroscopy

A team of researchers explore how time-domain spectroscopy can benefit from a well-designed sampling scheme. The proposed strategy leads to much shorter acquisition times while preserving the spectroscopic information content.

June 11, 2024

Optical spectroscopy is at the core of light-matter interaction. Modern ultrafast spectroscopy typically exploits broadband lasers with the pulse delay scanned in the time-domain. This research field, called time-domain spectroscopy, finds applications in material characterization (which, in turn, can be relevant for areas as diverse as chemistry, biology or energy), sensing or molecular classification, among others.

In general, one needs to sample a sufficient number of time steps over a long enough time range to capture the spectral response as a whole. The higher the number of samples, the more accurate reconstruction. As a downside, increasing this number requires longer data acquisition times, something that can become experimentally unfeasible, especially in more complex multidimensional spectroscopies. As surprising as it may seem, little attention to the sampling strategy has been paid within the field of spectroscopy, where generally only uniform or random distributions tend to be considered.

Now, with the aim of collecting data more effectively, ICFO researchers **Dr. Luca Bolzonello** and **Prof. ICREA Niek van Hulst**, together with Andreas Jakobsson from Lund University, have introduced a **systematic approach to optimize the sampling scheme in time-domain spectroscopy experiments**. The results, published in The Journal of Chemical Physics, show how, in stark contrast with the inefficiency of traditional sampling methods, their technique can significantly reduce the acquisition time while maintaining or even enhancing the quality of the data collected.

According to Dr. Luca Bolzonello, first author of the article, i¿½this optimization not on y saves time, but also reduces costs, minimizes sample degradation, and improves the overa l efficiency of experimental setupsi?

Optimizing the sampling scheme

The goal of the study was to find the balance between getting the maximum possible information and carrying out the minimum number of data acquisitions. The proposed

method exploits the prior knowledge of the spectroscopist performing the experiment to optimize the sampling scheme, as this foreknowledge avoids the collection of noisy data points with low information content.

More technically, researchers make use of the so-called Fisher information. Roughly speaking, the Fischer parameter matrix quantifies how much one can learn about a parameter based on the chosen sampling scheme and the noise of the experiment. i¿½ t turns out that this allows us to estimate the final uncertainty of measurements before th y are even takeni¿½, explains Bolzonello. i¿½By focusing on the most informative points, e can reduce the number of samples needed while still getting accurate and precise par meter estimates. This approach systematically enhances the quality of the data collected, aking the experiments more efficient and informati

ei¿½. The technique was benchmarked with several case studies, showcasing its pote tial to benefit the spectroscopic research. Now the team plans to implement this o timized sampling technique in a broader range of spectroscopic experiments to vali ate its effectiveness across different applications. In particular, classification of fluorescent ignals, material characterization and the study of molecular ultrafast dynamics are the areas t at will benefit t

Bibliographic reference:

Bolzonello L, van Hulst NF, Jakobsson A. Fisher information for smart sampling in time-domain spectroscopy. J Chem Phys. 2024 Jun 7;160(21):214110. doi: https://doi.org/10.1063/5.0206838