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A single-molecule FRET data fitting package for DNA folding kinetic study

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Single-molecule Förster (or fluorescence) resonance energy transfer is a commonly used biophysical technique to study DNA and protein folding dynamics. When two fluorescent dyes that have spectral overlap are placed nearby each other, energy will transfer from one dye to the other via the vibrating electric field very much like an induction coil for electricity transfer. This phenomena can be measured using a FRET microscope at the single-molecule level with a millisecond time-resolution that enables various of measurements for DNA and protein folding.¹

The data analysis methods for a system with ON and OFF two-state transitions have been well developed in the literature but it has been challenge for complicated systems involving transitions among many states.² Particularly, state identification is greatly affected by the camera blurring effect especially when the total transition speed approaching the integration time, and pulling out the rate constants from such data is also challenging due to the difficulty of fitting a system with many local minima.

The PI will introduce a software package he has developed to analyze such data.³ Briefly, the package is developed using MATLAB with an L1 norm random search algorithm. The data fitting is achieved from comparison between Monte Carlo simulated data and the experimental data using pattern recognition to reduce the effect of noise and camera blurring effect. The PI believes that this package will be useful for many researchers in NIDA genome study section that are working on DNA or protein dynamics and is transferable to other systems.

¹ J. Chen, ..., C.F. Landes, Single-Molecule FRET Studies of HIV TAR–DNA Hairpin Unfolding Dynamics, *JPCB*, 2014, 118(42), 12130-12139.

² M. Götz, ..., J. Chen, ..., S. Schmid, A blind benchmark of analysis tools to infer kinetic rate constants from single-molecule FRET trajectories, *Nat. Commun.*, 2022, 13, 5402.

³ J. Chen, ..., C.F. Landes, A Two-Step Method for smFRET Data Analysis, 2016, 120(29), 7128-7132.