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Spectral Multi Exponential Approximation as a Robust Tool for Analysis of Complex Systems

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The behavior of various systems in living and nonliving matter may be characterized mathematically by a linear combination of exponential functions. Many types of scientific experiments are often conducted in such a way that changes in some characteristic variable in response to some perturbation are recorded. These measurements yield data referred to as a signal. Assuming the signal by its nature is a linear combination of exponential functions, each of them characterizing response of particular subsystem to the perturbation, the researcher faces a task to find parameters (amplitudes and characteristic times) of particular exponential functions constituting the signal. There is no common method to find these parameters in general case because the problem is ill-conditioned.

In particular cases the task may be solved by linear regression. We develop the method of spectral multi-exponential approximation (SMEA) [Plyusnina et al., 2015], in which characteristic times of exponential functions are taken over fixed logarithmic scale, and non-negative least square solver is used to find pre-exponential factors. These factors (amplitudes) constitute discrete spectrum. To obtain scale-independent transform, for any arbitrary characteristic time we define the integral amplitude as a partial sum of estimated amplitudes corresponding to characteristic times less than this arbitrary time. Integral amplitude is a step function, and its plot against time provides a pictorial representation of the SMEA transform. A heatmap visualization of the integral amplitude with characteristic times coded by color is suitable for representation of a large sample of signals.

This method was applied for analysis of chlorophyll fluorescence transient in ecological and biotechnological studies. The measurement of the kinetics of chlorophyll fluorescence transient of algae and plants is a widely used method for determining the state of photosynthetic apparatus. The time dependence of the fluorescence intensity is a complex multiphase curve, which depicts the various stages of the electron transfer in the electron transport chain of chloroplasts. SMEA allows to formalize phase identification, to estimate quantitative characteristics of individual phases of the induction curve (amplitudes and characteristic times), and to reveal hidden phases of the curve. Occurrence of additional phases on the induction curve points to a change in the functioning of the photosynthetic apparatus in response to changing growth conditions. A high sensitivity of SMEA allows to suggest it for detection of early cell response to stress. SMEA decomposition and visualization techniques may find broad application in various signal processing tasks, especially in the analysis of the response of complex biological systems to external impact.

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References

Plyusnina, T.Y., Khrushev, S.S., Riznichenko, G.Y. et al. BIOPHYSICS (2015) 60: 392. doi:10.1134/S000635091503015X

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