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Fast heuristic method to bypass the numerical integration bottleneck when fitting non-linear differential equations

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Abstract

Fitting a model of nonlinear differential equations to a set of experimental data is a mathematical and computational problem that any scientist in any field of study may encounter. The standard approach to solving it involves repeated numerical integration of the differential equations, followed by a comparison of the theoretical and observed time trajectories, and then applying the appropriate fitting method. However, this brute-force procedure can be computationally very expensive, especially in huge systems that require precise temporal resolution and a large number of parameters to be fitted.

Thus, we present DILF (Derivative-Interpolation Least-squares Fitting), a method for fitting differential equations that completely bypasses the bottleneck of iterative numerical integration. In the DILF method, we approximate the empirical time series with auxiliary functions (selected via cross-validation). We then compare the analytical derivatives of these auxiliary functions with the velocity fields given by the theoretical model at the observed data points. By reformulating the problem in this way, the computationally expensive step of iterative integration is replaced by a simple algebraic evaluation, allowing for rapid adjustment of the model parameters using standard optimization methods. We have applied DILF to a wide range of problems using real experimental data from, among others, coupled ecological competition models and linguistic competition models. We then assessed the method's sensitivity to different model formulations, chaotic regimes, and redundant parameters.

DILF provides a practical, general-purpose tool for researchers who need to efficiently fit large models of nonlinear differential equations to empirical data without requiring advanced computational resources, thereby overcoming the main bottleneck associated with these methods.

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