Abstract Submitted
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Automated Probing and Inference of Analytical Models for Metabolic Network Dynamics[1] JOHN WIKSWO, Vanderbilt University, MICHAEL SCHMIDT, Cornell University, JERRY JENKINS, Hudson Alpha Institute, JONATHAN HOOD, CFD Research Corp, HOD LIPSON, Cornell University — We introduce a method to automatically construct mathematical models of a biological system, and apply this technique to infer a seven-dimensional nonlinear model of glycolytic oscillations in yeast – based only on noisy observational data obtained from *in silico* experiments. Graph-based symbolic encoding, fitness prediction, and estimation-exploration can for the first time provide the level of symbolic regression required for biological applications. With no *a priori* knowledge of the system, the Cornell algorithm in several hours of computation correctly identified all seven ordinary nonlinear differential equations, the most complicated of which was $\frac{dA_3}{dt} = -1.12 \cdot A_3 - \frac{192.24 \cdot A_3 S_1}{1+12.50 \cdot A_3^4} + 124.92 \cdot S_3 + 31.69 \cdot A_3 S_3$, where A_3 = [ATP], S_1= [glucose], and S_3 = [cytosolic pyruvate and acetaldehyde pool]. Errors on the 26 parameters ranged from 0 to 14.5%. The algorithm also automatically identified new and potentially useful chemical constants of the motion, *e.g.* $-k_1 N_2 + K_2 v_1 + k_2 S_1 A_3 - (k_4 - k_5 v_1) A_3^4 + k_6 \approx 0$. This approach may enable automated design, control and analysis of wet-lab experiments for model identification/refinement.

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