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Potterswheel Is a Matlab Toolbox for Mathematical Modeling of Time-Dependent Dynamical Systems That Can Be Expressed As Chemical Kinetics

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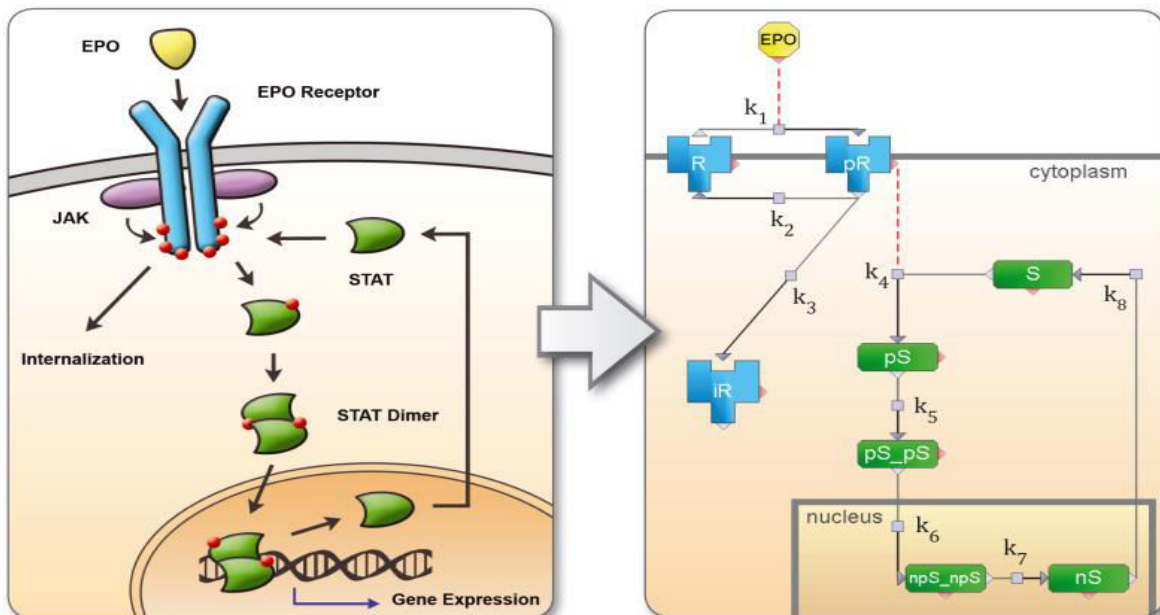
ABSTRACT: Potters Wheel is a MATLAB toolbox for mathematical modeling of time-dependent dynamical systems that can be expressed as chemical reaction networks or ordinary differential equations (ODEs).^[1] It allows the automatic calibration of model parameters by fitting the model to experimental measurements. CPU-intensive functions are written or – in case of model dependent functions – dynamically generated in C. Modeling can be done interactively using graphical user interfaces or based on MATLAB scripts using the PottersWheel function library. The software is intended to support the work of a mathematical modeler as a real potter's wheel eases the modeling of pottery.

KEYWORDS: Potters wheel, MATLAB, chemical reaction, modeling, mathematical, intensive, dynamical

I. INTRODUCTION

The basic use of PottersWheel covers seven phases from model creation to the prediction of new experiments.

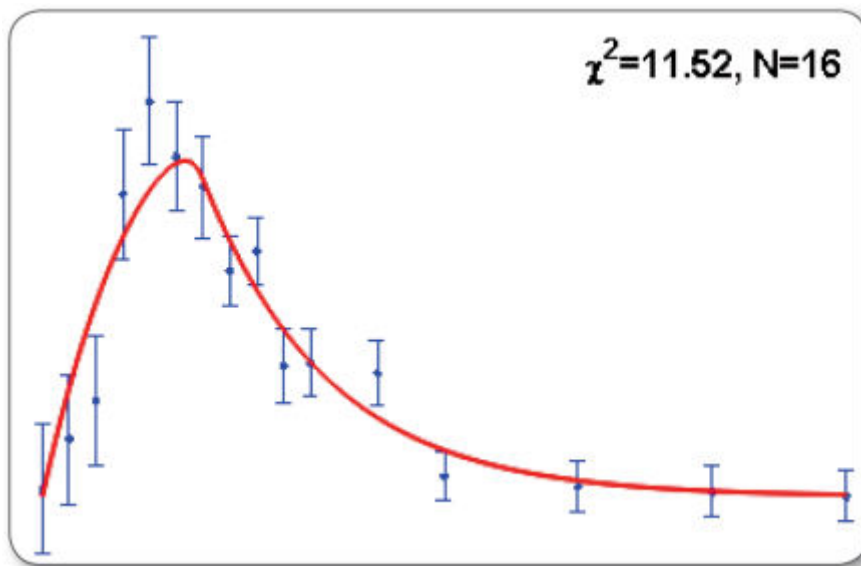
Model creation



The dynamical system is formalized into a set of reactions or differential equations using a visual model designer or a text editor.¹ The model is stored as a MATLAB *.m ASCII file. Modifications can therefore be tracked using a version control system like subversion or git. Model import and export is supported for SBML. Custom import-templates may be used to import custom model structures. Rule-based modeling is also supported, where a pattern represents a set of automatically generated reactions. External data saved in *.xls or *.txt files can be added to a model creating a model-data-couple. A mapping dialog allows to connect data column names to observed species names. Meta information in

the data files comprise information about the experimental setting. Measurement errors are either stored in the data files, will be calculated using an error model,² or are estimated automatically. To fit a model to one or more data sets, the corresponding model-data-couples are combined into a fitting-assembly. Parameters like initial values, rate constants, and scaling factors can be fitted in an experiment-wise or global fashion.³ The user may select from several numerical integrators, optimization algorithms, and calibration strategies like fitting in normal or logarithmic parameter space.

Interpretation of the goodness-of-fit



The quality of a fit is characterized by its chi-squared value. As a rule of thumb, for N fitted data points and p calibrated parameters, the chi-squared value should have a similar value as $N - p$ or at least N . Statistically, this is expressed using a chi-squared test resulting in a p -value above a significance threshold of e.g. 0.05. For lower p -values, the model is⁴

- either not able to explain the data and has to be refined,
- the standard deviation of the data points is actually larger than specified,
- or the used fitting strategy was not successful and the fit was trapped in a local minimum.

Apart from further chi-squared based characteristics like AIC and BIC, data-model-residual analyses exist, e.g. to investigate whether the residuals follow a Gaussian distribution. Finally, parameter confidence intervals may be estimated using either the Fisher information matrix approximation or based on the profile-likelihood function, if parameters are not unambiguously identifiable.⁵

If the fit is not acceptable, the model has to be refined and the procedure continues with step 2. Else, the dynamic model properties can be examined and predictions calculated.

If the model structure is not able to explain the experimental measurements, a set of physiologically reasonable alternative models should be created. In order to avoid redundant model paragraphs and copy-and-paste errors, this can be done using a common core-model which is the same for all variants. Then, daughter-models are created and fitted to the data, preferably using batch processing strategies based on MATLAB scripts. As a starting point to envision suitable model variants, the PottersWheel equalizer may be used to understand the dynamic behavior of the original system.⁶

II. DISCUSSION

A mathematical model may serve to display the concentration time-profile of unobserved species, to determine sensitive parameters representing potential targets within a clinical setting, or to calculate model characteristics like the half-life of a species.

Each analysis step may be stored into a modeling report, which may be exported as a Latex-based PDF.⁷

An experimental setting corresponds to specific characteristics of driving input functions and initial concentrations. In a signal transduction pathway model the concentration of a ligand like EGF may be controlled experimentally. The driving input designer allows investigating the effect of a continuous, ramp, or pulse stimulation in combination with varying initial concentrations using the equalizer. In order to discriminate competing model hypotheses, the designed experiment should have as different observable time-profiles as possible. Many dynamical systems can only be observed partially, i.e. not all system species are accessible experimentally. For biological applications the amount and quality of experimental data is often limited. In this setting parameters can be structurally or practically non-identifiable. Then, parameters may compensate each other and fitted parameter values strongly depend on initial guesses. In PottersWheel non-identifiability can be detected using the Profile Likelihood Approach.^[2] For characterizing functional relationships between the non-identifiable parameters PottersWheel applies random and systematic fit sequences.⁸

Ordinary differential equations (ODEs) arise in many contexts of mathematics and social and natural sciences. Mathematical descriptions of change use differentials and derivatives. Various differentials, derivatives, and functions become related via equations, such that a differential equation is a result that describes dynamically changing phenomena, evolution, and variation. Often, quantities are defined as the rate of change of other quantities (for example, derivatives of displacement with respect to time), or gradients of quantities, which is how they enter differential equations.

Specific mathematical fields include geometry and analytical mechanics. Scientific fields include much of physics and astronomy (celestial mechanics), meteorology (weather modeling), chemistry (reaction rates),^[3] biology (infectious diseases, genetic variation), ecology and population modeling (population competition), economics (stock trends, interest rates and the market equilibrium price changes).⁹

Many mathematicians have studied differential equations and contributed to the field, including Newton, Leibniz, the Bernoulli family, Riccati, Clairaut, d'Alembert, and Euler.

III. RESULTS

A solution that has no extension is called a maximal solution. A solution defined on all of \mathbb{R} is called a global solution.¹⁰

A general solution of an n th-order equation is a solution containing n arbitrary independent constants of integration. A particular solution is derived from the general solution by setting the constants to particular values, often chosen to fulfill set 'initial conditions or boundary conditions'.^[18] A singular solution is a solution that cannot be obtained by assigning definite values to the arbitrary constants in the general solution.^[19]

In the context of linear ODE, the terminology particular solution can also refer to any solution of the ODE (not necessarily satisfying the initial conditions), which is then added to the homogeneous solution (a general solution of the homogeneous ODE), which then forms a general solution of the original ODE. This is the terminology used in the guessing method section in this article,^[1] and is frequently used when discussing the method of undetermined coefficients and variation of parameters. The theory of singular solutions of ordinary and partial differential equations was a subject of research from the time of Leibniz, but only since the middle of the nineteenth century has it received special attention. A valuable but little-known work on the subject is that of Houtain (1854). Darboux (from 1873) was a leader in the theory, and in the geometric interpretation of these solutions he opened a field worked by various writers, notably Casorati and Cayley^[12]. To the latter is due (1872) the theory of singular solutions of differential equations of the first order as accepted circa 1900. The primitive attempt in dealing with differential equations had in view a reduction to quadratures. As it had been the hope of eighteenth-century algebraists to find a method for solving the general equation of the n th degree, so it was the hope of analysts to find a general method for integrating any differential equation. Gauss (1799) showed, however, that complex differential equations require complex numbers. Hence, analysts began to substitute the study of functions, thus opening a new and fertile field. Cauchy was the first to appreciate the importance of this view. Thereafter, the real question was no longer whether a solution is possible by means of known functions or their integrals, but whether a given differential equation suffices for the definition of a function of the independent variable or variables, and, if so, what are the characteristic properties. Two memoirs by Fuchs^[13] inspired a novel approach, subsequently elaborated by Thomé and Frobenius. Collet was a prominent contributor beginning in 1869. His method for integrating a non-linear system was communicated to Bertrand in 1868. Clebsch (1873) attacked the theory along lines parallel to those in his theory of Abelian integrals. As the latter

can be classified according to the properties of the fundamental curve that remains unchanged under a rational transformation, Clebsch proposed to classify the transcendent functions defined by differential equations according to the invariant properties of the corresponding surfaces $f = 0$ under rational one-to-one transformations. From 1870, Sophus Lie's work put the theory of differential equations on a better foundation. He showed that the integration theories of the older mathematicians can, using Lie groups¹⁴, be referred to a common source, and that ordinary differential equations that admit the same infinitesimal transformations present comparable integration difficulties. He also emphasized the subject of transformations of contact.¹⁴

Lie's group theory of differential equations has been certified, namely: (1) that it unifies the many ad hoc methods known for solving differential equations, and (2) that it provides powerful new ways to find solutions. The theory has applications to both ordinary and partial differential equations.¹⁶ A general solution approach uses the symmetry property of differential equations, the continuous infinitesimal transformations of solutions to solutions (Lie theory).²⁹ Continuous group theory,²⁸ Lie algebras, and differential geometry are used to understand the structure of linear and non-linear (partial) differential equations for generating integrable equations, to find its Lax pairs, recursion operators, Bäcklund transform, and finally finding exact analytic solutions to DE. Symmetry methods have been applied to differential equations that arise in mathematics, physics, engineering, and other disciplines.¹⁵

IV. CONCLUSIONS

When all other methods for solving an ODE fail, or in the cases where we have some intuition about what the solution to a DE might look like, it is sometimes possible to solve a DE simply by guessing the solution and validating it is correct.³⁰ To use this method, we simply guess a solution to the differential equation, and then plug the solution into the differential equation to validate if it satisfies the equation. If it does then we have a particular solution to the DE, otherwise we start over again and try another guess. For instance we could guess that the solution to a DE has the form. Since this is a very common solution that physically behaves in a sinusoidal way.³¹

In the case of a first order ODE that is non-homogeneous we need to first find a DE solution to the homogeneous portion of the DE, otherwise known as the characteristic equation, and then find a solution to the entire non-homogeneous equation by guessing. Finally, we add both of these solutions together to obtain the total solution to the ODE.³²

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