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Exploring an Engineering problem with uncertainty in an interdisciplinary journey on the Web

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Abstract: We present the study of a system of nonlinear ordinary differential equations (ODEs), and our objective is to tackle the problem under these complementary perspectives: (*i*) preliminarily, solving the IVP system of ODEs numerically; (*ii*) exploring the solution by imposing random variation on the initial values (IVs), subjected to Gaussian distributions; and (*iii*) providing a constructed, free web page for the consequent dynamic verification of our results by the reader.

The study interlaces modeling and data analysis in an interdisciplinary context, combining a question in Engineering, its mathematical resolution, and its computational and operational research approaches, with a glance at Artificial Intelligence (AI).

The IVs are subjected to random variation, in order to assess the effect of the uncertainty on the quality of the results. Indeed, the IVs are data that can be inaccurate in contrast to the admittedly rigorous mathematical methods. Our problem is related to manufacturing, emanates from Chemical Engineering, and is treated in its mathematical nature, for greater generality.

If the data depend on a practical operation, this may introduce errors, all the more so if the operation is repetitive, hasty, such as in an industrial environment. The problem stems from chemical kinetics, and is adapted from the kinetics of an arbitrary "autocatalytic" reaction, suggested by AI.

The problem was chosen merely because the above mentioned reactions are typically described by nonlinear systems of ODEs that require numerical integration, which facilitates to solve most problems by nonspecialists, such as practicing engineers.

Regarding methodology, the study has two stages: (*i*) in a preparatory stage, we present the numerical resolution of the ODEs; and (*ii*) in the main stage, Monte Carlo simulation is applied to the said resolution under random variation of the IVs, in order to assess the effect of that variation under a certain criterion.

STAGE 1: the system of nonlinear ODEs is solved numerically by means of the Python procedure 'solve_ivp', allowing to use any of its methods (such as Runge-Kutta). The (free) languages chosen are: PHP to construct the web page; Python for computing, embedded in the web page; and 'gnuplot' (instead of the usual Python module 'matplotlib') as a graphical utility, adopted, once more, for generality, because it is easily called from languages (C, Fortran, etc.) without graphical capabilities.

Although this text is only an abstract of a full description, the result in this stage and the second —according to our Web strategy— can be seen in reference [2] (M. Casquilho, 2025. Explore ODEs, uncertainty), which contains a link to the computation, with all of its results.

STAGE 2; the criterion (among many) was to examine the behavior of the maximum of $y(t)$, one of $x(t)$, $y(t)$, $z(t)$, for the best instant, t^*, found in the previous stage. The maximum is attained only if the IVs are the correct ones, otherwise $y(t^*)$ will oscillate around the true value. How much it oscillates is the result of the study. The value of $y(t^*)$ will oscillate around the true maximum, as the evolution of the functions is affected by the perturbed IVs. These IVs are each made Gaussian, with μ its true value and $\sigma = c_v \mu$. Values of c_v, such as 0.5%, 1%, 2%, 5%, 10%, reveal expected increasing distance from the true maximum. The statistical behavior of this value approaches Gaussians, finding their parameters being out of our scope. Interestingly, a finer analysis from extensive Monte Carlo runs negates this impression, by showing a slight positive skewness.

The computations led to qualitative variability in the results, which would, without the proposed procedure, be quantitatively unpredictable.

Providing a Web route to verify our results is meant to be one of the novelties in the study. The web page can be used with our default data or other supplied by a user. This mode of operation is also a gateway for the desired link between academia and industry.

In sum, we studied a system of ODEs describing the dynamics in a Chemical Engineering problem, to assess

its behavior under uncertainty in the IVs of the ODEs. This was achieved by Monte Carlo simulation, combining Engineering, Mathematics (with Statistics and Operational Research), Computing, and an aid from Artificial Intelligence, and resulting in a constructed, dynamic web page.

We have since long adopted the Web as a computing medium, using terms such as "web-computing" (references to our work in 2011–2024), although this preference seems rare in the literature (an exception by Ponce's academic website). Regarding journal articles, the presence of links to computing web pages is rare. Programs sometimes are offered in repositories in languages unknown to the reader. We have advocated our mode of sharing and promoting connectivity, which itself simultaneously protects the authors' own labor.

The accommodation to the Web does not fare without its perils. In fortuitous articles with links for verification, the links land on extinct addresses. If we recall *verba volant, scripta manent*, any article or similar invoking links to direct computations must survive, maintaining its value, even if the linked addresses disappear. In the present and other articles, we comply with this principle by inserting all the related information. The advantage of the Web as the computing medium is the possibility offered for the user to confirm the results shown and try other data. This opening is friendly and has the handy advantage of immediacy.

Keywords: modeling; web computing; ordinary differential equations; Monte Carlo simulation; Engineering.

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