Initial Estimates for Parameter Estimation: Integration Free Parameter Estimation

Vivek Dua (v.dua@ucl.ac.uk)

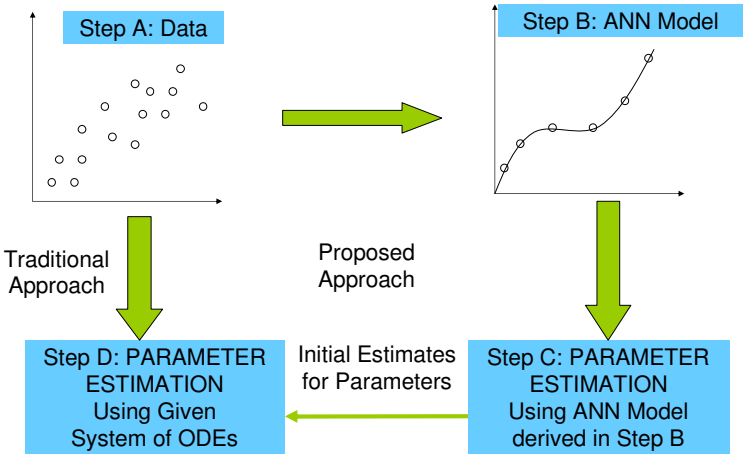
Centre for Process Systems Engineering, Department of Chemical Engineering,
University College London, Torrington Place, London, WC1E 7JE.

Background, Motivation and Objectives

Parameter estimation for models involving differential equations corresponds to a dynamic optimization problem, which in general has multiple locally optimal solutions. The solution techniques for global optimization can be broadly classified as deterministic and non-deterministic methods. Deterministic methods can guarantee that solution obtained is globally optimal within a certain pre-specified tolerance whereas the non-determinstic methods do not provide any such guarantee. However these methods are computationally demanding and most of the commercially available softwares for parameter estimation are based upon local optimization techniques. The main objective of this work is to develop algorithms for obtaining good quality initial estimates, which can speed-up the solution times, reduce solver failures, and increase possibility of obtaining the globally optimal solution.

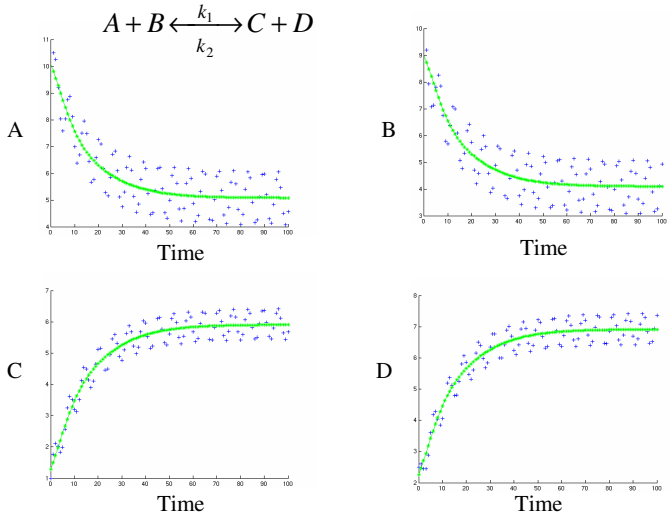
Proposed Methodology for Parameter Estimation

The parameter estimation problem is decomposed into two sub-problems. The first sub-problem corresponds to developing an Artificial Neural Network (ANN) model for the given data. The ANN model represents a reduced data set. The second subproblem is formulated as a parameter estimation problem where the differential terms in the model are obtained by analytically differentiating the ANN model. The second subproblem corresponds to a Linear Program (LP) or a Nonlinear Program (NLP), for which reliable solvers are available. The solution of the second subproblem provides initial estimates for parameters. These estimates are then used to solve the original parameter estimation problem.



$$\frac{dA}{dt} = \frac{dB}{dt} = -\frac{dC}{dt} = -\frac{dD}{dt} = -k_1.A.B + k_2.C.D$$

$$A + B \underset{k_2}{\overset{k_1}{\longleftrightarrow}} C + D$$



The data was generated by simulating the model for k_1 = 4E−3 and k_2 = 2E−3 and then adding noise to the data. By using the proposed methodology the ANN approximation of the model was obtained (shown as green line). This approximation was then used to estimate the parameters, and the solution was given by k_1 = 4.132E−3 and k_2 = 2.195E−3. No integration of differential equations was carried out for parameter estimation!

Conclusions

The main advantage of using the proposed decomposition approach is that the error between the data and model predictions is minimized in the first step and the parameter estimation for a reduced data set is carried out in the second step. ANN is well known for its ability to handle large data sets and characterize highly nonlinear functions very effectively. This ability together with the differentiability properties of ANN makes the proposed approach a very useful tool for parameter estimation of problems involving differential equations and large data sets.