Parameter Fitting : which algorithm to choose ?

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PARAMETER FITTING: WHICH ALGORITHM TO CHOOSE ?

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Introduction

Hydrocracking (HCK) is one of the most versatile petroleum refining processes. It usually converts a heavy, low quality feedstock (VGO: Vacuum Gas Oil) into lighter, valuable transportation fuels, contributing significantly to the overall profitability of the refinery [1]. A robust kinetic model allows the optimal process design and operating conditions to be chosen to maximize the desired cuts and product characteristics. Hydrocracking of VGO residue performed in a two-step process: 1) a hydrotreatment step in the first reactor, which serves mainly to remove nitrogen and sulfur from the feed; 2) a hydrocracking step in the second reactor, which performs the main hydrocracking reactions on a zeolite-type catalyst. A kinetic model is defined by its structure and its parameters, which are estimated from collected data. The main difficulty is the parameter fit on real data. The aim of this paper is to compare several optimization algorithms on a continuous lumping model of the hydrocracking step. It is structured as follows:

- Case study description,
- Description of the chosen optimization algorithms,
- Results.

Case study: hydrocracking

The experimental runs presented in this study were performed in a pilot plant at IFP Energies Nouvelles, Solaize, France. The hydrocracking step was performed on a commercial zeolite cracking catalyst. The plant consists of a number of fixed beds, up-flow reactors, designed to mirror the operating conditions in industrial hydrocracking units. A series of mass balances with different operating conditions is thus taken from each experimental run. Each mass balance corresponds to a single experimental point.

Analyses were performed on the feedstocks, the liquid and gaseous effluents. The most relevant measurements in this study were the feed sulfur and nitrogen contents, the partial pressures of NH_3, H_2S, and H_2 gasses, as well as the simulated distillation (SIMDIS).

A calibration database, consisting of 29 mass balances, was compiled. This database was used for the identification of the empirical parameters in a continuous lumping model originally developed for the first reactor but extended to the second one [2]. The range of the main operating conditions, temperature and liquid hourly space velocity (LHSV) is classical: $T \in [370;400°C]$, $LHSV \in [0.5;3\ h^{-1}]$. The conversion of the 370°C fraction (X370+) is between 50 to 90%w/w.

Optimization method tested

The parameter fit problem is formulated as the following least-square minimization problem

$$\min_{l \le x \le u} \sum_{i=1}^{N_d} \left(\frac{\boldsymbol{m_i(x) - d_i}}{\boldsymbol{\sigma_i}} \right)^2 \qquad (1)$$

with

- x, vector of model parameters to be tuned,
- l, u, lower and upper bounds of x,
- N_d, size of experimental data,
- $m_i(x) \in \mathbb{R}^{N_d}$, vector of simulated data to be compared with experimental data,
- $d_i \in \mathbb{R}^{N_d}$, vector of experimental data to be fit,
- σ_i, weights modeling the measure uncertainties.

This optimization problem belongs to the class of derivative free or black-box optimization problems. Indeed, the simulator associated with the kinetic model computes the simulated data to be compared with experimental ones but does not provide the associated derivatives with respect to the parameters. Classical optimization methods, namely gradient based methods, require those derivatives: therefore, when they are not available as simulator outputs, they are usually estimated by finite difference scheme, which requires NP simulations for each gradient computation (NP being the number of parameters). The associated computational cost may thus become too high when the number of parameters increases. Moreover, the tuning of the perturbation step may be cumbersome in practice when numerical noise is present in the simulation.

An alternative is derivative free optimization methods which have become very popular with the emergence of adapted trust region methods [3,4]. SQA, developed by [5] at IFPEN, is a trust region method coupled with interpolating quadratic models. It has been applied successfully on several industrial applications [6,7] and has shown better performances than gradient based methods with finite difference estimate of derivatives. This method is an extension of the method proposed by Powell in [3] to nonlinear constrained problems. The main principle of the method is the following: in order to save simulations, quadratic interpolating models are used as surrogate of the simulator responses. These quadratic models are minimized and updated thanks to additional simulations performed along the optimization process iterations. For least-square formulations, the quadratic models approximate the residuals (differences between experimental and simulated data) instead of the single objective function, in order to improve the accuracy of the approximation.

In the following section, SQA method is compared to the Gauss-Newton method implemented in Port library (DN2FB method) [8]. For this latter method, the Jacobian matrix (derivatives of simulated data with respect to parameters) is estimated by finite differences.

Results

The performances of the SQA and Port algorithms for the Hydrocracking model parameter identification have been compared. The continuous lumping model requires a total of NP=28 experimental parameters to be identified. A target function, based on the yield structure (standard cuts: <150°C, 150-250°C, 250-370°C, >370°C and C1-C4 gas) is defined. The same target function and initial parameters were used for both algorithms.

The SSQ is decreased by an order of magnitude, from 1.7×10^9 to 4.1×10^8 by the Port algorithm and to 4.2×10^8 by the SQA algorithm. The evolution of the sum of square residuals with the number of function evaluations for the SQA and Port (DN2FB) algorithms are shown in figure 2. Both methods attain a minimum. The gradient base method (DN2FB) reached a minimum after around 240 function calls. The response-surface based method (SQA) reached a minimum after 190 function calls. The decrease of the SSQ is very gradual for the DN2FB algorithm. The SQA algorithm first constructs the interpolation of the response surface for a total of 2xNP+1 = 57 function calls. This is characterized by an exploration phase around the initial value of the SSQ. Once the response surface has been constructed, the algorithm rapidly descends towards the minimum (about 60 function calls). The baseline of the SSQ does not decrease significantly after this step. A number of oscillations can be observed, as the algorithm refines the search for the local minimum.

Both of the local optimization algorithms, DN2FB and SQA are found to converge to a local minimum with the same square residual. The trust-region method (SQA) shows better performance on the test case than the gradient based-method with finite difference approximation (DN2FB). Once the response surface has been constructed (i.e. exploration around initial point in Figure 1), the SQA algorithm rapidly attains the local minimum. The DN2FB algorithm decreases the residuals much more gradually. Furthermore, the parameter space is explored much more thoroughly by the SQA algorithm, which is illustrated by the large spikes in Figure 1. The finite difference algorithm perturbs only slightly the parameters around each iterate for gradient estimation. This feature makes SQA less likely to be caught in a local minimum.

Conclusion

This paper compares two optimization methods for fitting kinetic model parameters. In this example, the SQA method proves to be more efficient than classical gradient method.

The fact that two different sets of parameters yield to the same sum of square residuals suggests the presence of local minima. Adding chemical/physical *a-priori* information can help to constrain the system and to remove this under-determination.

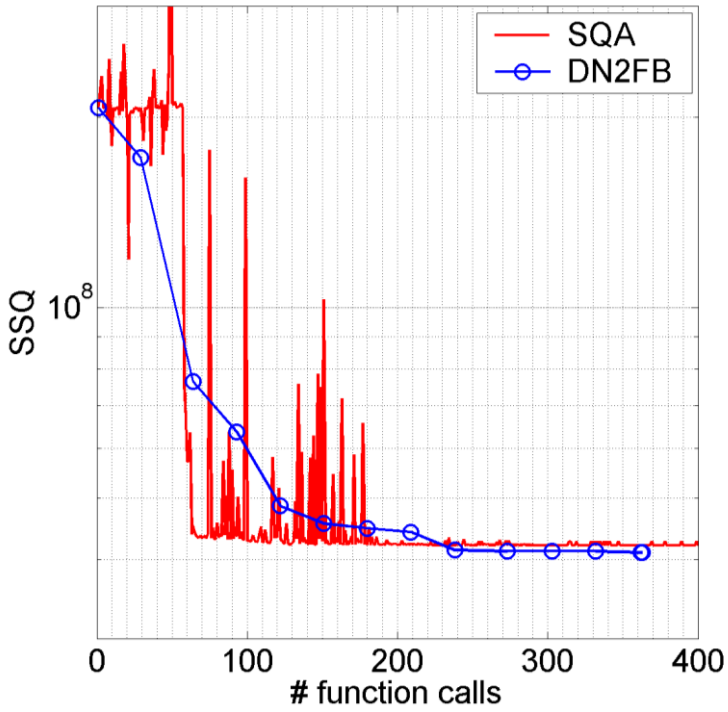

Figure 1 : Sum of Square Residuals (SSQ) with function evaluations for SQA and Port (DN2FB) algorithms

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