# On the integration of optimization and stability: the matrix measure relaxation method and its application to the optimal synthesis of complex nonlinear systems.

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## Abstract

Keywords: Stability, optimization, measure relaxation, modeling, nonlinear networks.

Addressing stability and optimization issues simultaneously is a major challenge for most engineering processes in which nonlinear dynamical systems are integrated in the process flowsheet through a stream network of feedforward and backward interconnections. The stabilization of an engineering process is often attained by manipulating the operating parameters of the system and it almost always disregards the large number of structural alternatives one may take advantage of. In a process flowsheet, alternatives of this type include the potential rearrangement of the connectivity, reallocation or conversion of the utilities, as well as the consideration of unit bypassing and recycling. The problem is even more critical when the system is studied at a synthesis level where the optimization problem is to reveal the advantageous flowsheet of the process. Powerful generalized structures, better known as superstructures, are invoked to identify the synthesis alternatives and accommodate for an exhaustive superposition of all the design options. However, the

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superstructure layout remains unexploited due to the absence of a rigorous methodology which is capable of explicitly embedding the stability concerns in the large-scale mathematical formulations it always results to. Disregarding stability, the solution of the problem reveals configurations and operating points which, although optimal do not, in general, represent stable operaing points. In the case of inexpensive control action and/or perfect controlability, such an unstable solution may still be the desired alternative for the process. There are cases, however, for which either the controlability over the process is limited or one is interested in studying the tradeoffs between the unstable optimal solution and an optimal stable one.

A typical engineering problem whose study and analysis is always associated with stability problems is the optimal synthesis of a nonisothermal chemical reactor. The general character of the steady state operation of the continuous stirred tank reactors have been systematically studied in the last two decades and a large number of theoretical studies have been performed focused on the development of phase portrait and bifurcation diagrams (Uppal et al: 1974, 1976, Dangelmayr and Stewart: 1982), as well as on identifying various uniqueness and multiplicity criteria (Luss and Balakotaiah: 1982, 1985, 1987). Most of these criteria are based upon the singularity theory which has introduced a systematic framework with interesting results. However, the theory is applicable only to models described by a single intrinsic variable and provides local results given, at least in the majority of cases, in an implicit form. Thus, the application of these criteria for design purposes is all but possible and, since ignition and extinction problems may seriously endanger the operation of the reactors, conservative mechanisms are often invoked (Westerterp and Westerink: 1991) which move the unit performance into extremely suboptimal points. If, instead, the overall performance could be coupled with the stability concerns, the optimization of the system would reveal advantageous structural and operational alternatives.

The motivation behind the work presented in this paper has primarily been to develop a systematic framework in order to meet stability concerns for the optimal solutions obtained in the design of processes modeled by nonlinear systems. The focus is on addressing the general problem rather than special cases of it, as well as on accommodating for large-scale implementations. The system in question involves variables and undetermined parameters which are to be specified by optimizing the process based upon a given performance criterion. Although at the assumed analysis level neither the eigenvalues of the linearized system can be calculated nor eiher one the Lyapunov's direct and indirect methods is applicable, the desired methodology has to systematically lead toward a stable operating point. For this purpose a systematic approach is proposed by defining and implementing an iterative algorithmic procedure. The approach identifies a stable and unstable domain, introduces the notion of the matrix measures in the variable space of the problem, and augments the null space of the mathematical formulation with relaxation parameters. The relaxation parameters are initialized based upon the solution of the original formulation and are upgraded throughout the execution of the algorithmic procedure. The procedure is based upon the iterative solution of optimization problems in the stable and unstable domain. The solution in the stable domain provides a lower bound for the final solution while each solution in the unstable domain provides an upper bound. The relaxation parameters are successively updated in each case and iterations continue until the lower bound sufficiently approaches or exceeds the upper bound.

The augmentation of the initial formulation involves only convex constraints and does not complicate the solution or its optimality. Furthermore, the methodology is not restricted by the size of the problem nor is assuming special types of nonlinearities. It can be extended to arbitrarily large systems and only assumes the existence of a feasible stable solution. The potential of the approach is illustrated with two example problems pertaining to the optimal synthesis of complex networks. The networks are comprised by nonisothermal chemical reactors with the potential to be heated or cooled, and/or be operated in a desired range of the available parameter space. Furthermore, the units are interconnected in all possible ways thus resulting to a general unit superstructure. Cases of units arranged in either series or parallel or series-parallel configurations can all be obtained as special cases of the superstructure scheme. Moreover, all reactors are potentially recycled and/or bypassed. In both examples the methodology is applied to the entire superstructure scheme which it rigorously optimizes for the best stable operating point. The objective functions are described in terms of linear and/or nonlinear functions and the nonlinearities involve exponential and inverse terms as well as other multilinearities (bilinearities and trilinearities). Implementation of the methodology required less than 10 iterations and the solution revealed both structural and operational alternatives that stabilize the operation of the system and result into the best possible performance.