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Final Report

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Modeling for Process Control

Manfred Morari
Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena, California 91125
phone (818) 395-4186
fax (818) 568-8743
e-mail Morari@CALTECH.EDU

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MOTIVATION

Explosive developments have taken place in the control field during the last decade. In the context of this work, we will mention three of these milestones: first, the industrial development and application of *model predictive control* (MPC), a technique especially suitable for multivariable highly interactive processes involving constraints on manipulated as well as controlled variables. Second, on the theory side, *robust control* emerged as the eminent paradigm. Robust control aims at analyzing the effects of model uncertainty on closed loop performance and to incorporate insensitivity to model uncertainty into the control system design procedure in a systematic fashion. And third, substantial advances have been made in the mathematical theory of the dynamics of *nonlinear systems*. Various nonlinear control techniques have grown out of this work which have excellent potential to address some difficult and long-standing process control problems.

While these developments received much publicity and attracted widespread interest, their impact on industrial control practice has fallen far short of their full potential. Many companies have expressed the desire to implement MPC schemes, but actual applications have been mostly limited to the major oil companies. The insights from robust control have proved valuable and have raised high expectations but only very few of the mathematical and control scientific discoveries have found their way into the control room.

The routine application of MPC and robust control faces many obstacles. *One key difficulty which stands in the way of these new as well as many other advanced control techniques is the need for a model to describe the dynamic behavior of the process to be controlled*. While many aspects of modeling have been studied for decades, the *modeling needs for control* purposes are largely not understood. It is not known how accurately the various system components have to be modeled so that a controller designed on the basis of the model works well on the real plant. Modeling is expensive and a clear understanding of the trade-offs between model accuracy and control quality is essential for assessing the economic viability of advanced control schemes. It is of key interest to minimize the modeling effort required for a specific control implementation.

Identification/modeling and control cannot be viewed as two independent activities: The type of model available determines the range of suitable control tools and vice versa, the type of robust control technique determines what model and uncertainty description is required. Thus, naturally work has to proceed on both identification and robust control design in parallel to reach an appropriate compromise between computational complexity of the robust control task and engineering relevance of the model/uncertainty description.

FINAL REPORT

Specifically, we have been pursuing 1) the development of linear regression techniques for problems with collinear data and 2) the development of tools for robust model predictive control system design for constrained and nonlinear systems; in particular, we are trying to establish what model uncertainty descriptions are suitable for design.

Linear Regressions Techniques for Problems with Collinear Data

Many practical modeling problems in a wide range of application areas including chemometrics, dynamic system identification, fault detection, etc. require at some stage the solution of a linear regression or linear least squares problem. Quite frequently the "normal equations" which define the solution of these problems are ill-conditioned. Physically this implies that the experimental data are not sufficiently rich to estimate all the model parameters accurately. The practical implication is that the parameter variances are large and that the parameter estimates are highly sensitive to the particular experimental data. All proposed approaches to deal with this problem trade off parameter variance against bias of the estimates. A very common approach is regularization (also referred to as ridge regression in the statistics literature) where a penalty term involving functions of the parameters to be estimated is added to the least squares objective. However, this approach is only meaningful if there is an underlying physical motivation to keep the parameters or some relation between the parameters (first or second difference) small.

Because this is often not the case, alternative approaches have been developed. Two popular ones are principal component regression (PCR) and partial least squares (PLS). In both cases the parameter vector to be estimated is projected down to a lower dimensional subspace. The key question is how that space is to be chosen based on the experimental data.

PLS was proposed more than a decade ago and is used widely in chemometrics, but it is not accepted by the orthodox statistics community because it lacks a rigorous statistical foundation, and the assumptions somehow implicit to the technique have never been stated. We succeeded in developing a new technique which we call significance regression. The subspace into which the (unknown) parameter vector is projected is developed successively via a hypothesis testing approach. In effect, the "significance" of the parameter estimates (where significance is defined as the ratio of the parameter estimate to its variance) is maximized. This new estimation approach has a number of attractive features.

- In the scalar output case, it is identical with PLS. Thus, it provides a consistent explanation for PLS which is attractive from a tutorial point of view. It also allows us to extend and interpret PLS in many interesting ways.

- We found that PLS is "statistically inconsistent" for the vector output case. The new technique (significance regression) does not suffer from the same deficiency. We showed it to lead to parameter estimates with reduced variance when compared to PLS.

- Typical assumptions inherent in ordinary least squares, in particular, that the inputs are known error free are often not satisfied. A significance regression technique for the so-called "measurement error model" was developed.

- It is known that ordinary least squares and its derivatives like PLS and PCR can suffer badly from the presence of data outliers. A new robust significance regression technique was developed, greatly alleviating this problem.

- While ordinary least squares is independent of input scaling, the various bias regression techniques like PLS, PCR and RR are not. New insights into the proper scaling of the input variables were obtained.

- Because of the statistical foundation of significance regression, it was possible to define statistical criteria for selecting the appropriate subspace dimension necessary to describe the parameter vector to be estimated. This test is a useful alternative to cross validation which is commonly practiced.

Robust Model Predictive Control System Design for Constrained and Nonlinear Systems

In the second part of the project we approach the problem area from the control side and try to establish the most general uncertainty descriptions for which robust stability and robust performance can be guaranteed with reasonable computational effort.

We developed the first numerically efficient technique for the robust control of linear multivariable systems in the presence of constraints. The allowed model uncertainty description (a function of the impulse response matrices) for which robust stability can be established, was identified. Some necessary and some sufficient conditions for robust stability were established elucidating the relationship between uncertainty and stability. The approach we are taking utilizes a number of tools from robust control theory and establishes stability via Lyapunov function arguments.

For a class of magnitude bounded uncertainties on the impulse response coefficients, we showed that the number of variables and constraints of the linear program which has to be solved on-line grows *linearly* with the problem dimensions. Thus, the required computational effort is exceptionally low and the technique is practical for reasonably large problems even for relatively high-speed applications.

We also addressed similar issues for general nonlinear systems. We developed an implementable technique for the robust control of nonlinear systems and identified the necessary model accuracy/allowed model uncertainty. The technique which falls into the category of receding horizon control has some unique features. In particular, for the on-line computations only a locally linearized model is employed greatly simplifying the computations. Also, stability guarantees for the output feedback case were established.

PROJECT OUTPUT

The project output falls into three categories: Publications, dissemination of the results through seminars and mini-workshops, and software.

Publications

The publications fall into three groups.

1. Publications related to regression.

1. T.R. Holcomb and M. Morari. Significance Regression: Robust Regression for Collinear Data. *Technometrics* (submitted); also *Proc. of American Control Conference*, San Francisco, CA, 1875-1879 (1993).

2. T.R. Holcomb, H. Hjalmarsson and M. Morari. Significance Regression: A Statistical Approach to Biased Regression and Partial Least Squares. *J. of Chemometrics* (submitted).

3. T.R. Holcomb and M. Morari. PLS Leads to Different Algorithms for Factor Analysis and Regression. *Chemometrics and Intelligent Laboratory Systems* (submitted).

4. T.R. Holcomb and M. Morari. Significance Regression: Improved Estimation from Collinear Data for the Measurement Error Model. *J. of the American Statistical Association* (submitted).

2. Publications related to model uncertainty.

5. C. Webb, H. Budman and M. Morari. Identification of Uncertainty Bounds for Robust Control with Applications to a Fixed Bed Reactor. *Int. J. of Control* (submitted).

6. A. Zheng and M. Morari. Robust Stability of Constrained Model Predictive Control. *Proc. of American Control Conference*, San Francisco, CA, 379-383 (1993).

7. A. Zheng and M. Morari. Robust Stability of Linear Systems with Constraints *Proc. of American Control Conference*, Baltimore, MD, xxx (1994).

8. S. L. de Oliveira and M. Morari. Stability and Robustness Properties of Model Predictive Control of Nonlinear Systems. *Proc. of IFAC Symposium on Robust Control Design*, Rio de Janeiro, Brazil, xxx (1994)

3. Publications of a more general nature.

9. M. Morari. Some Control Problems in the Process Industries. *Essays on Control: Perspectives in the Theory and its Applications*, H.L. Trentelman and J.C. Willems eds. Birkhäuser, Boston, 55-78 (1993). (Invited keynote lecture at European Control Conference 1993)

10. M. Morari. Current Directions in Process Control Theory. *Proceedings of PSE'94*, Fifth International Symposium in Process Systems Engineering, Kyongju, Korea, May 30-June 3, 1994. (Invited keynote lecture)

Seminars and Mini-Workshops

The results of this work were presented in seminars at various U.S. universities and at Shell Oil Company, Du Pont, Kodak and the Norwegian Technical University in Trondheim. The reaction of the statisticians, who constituted the major audience in the latter three instances, was overwhelmingly positive.

In February 1993 in direct connection with the DOE project, we organized an informal mini-workshop on process monitoring and diagnostics here at Caltech. Among the participants were Professor Karl Åström from Lund Institute of Technology in Sweden, a number of academics from Southern California universities and representatives from Avery-Dennison, Shell, Profimatics, Eastman Kodak, and DuPont. The purpose of this workshop was to give the people in industry an opportunity to present their problems and ideas and provide feedback to us on the progress of our work.

Software

The PLS identification technique was incorporated in the following commercial software package:

M. Morari and N. Lawrence Ricker. *Model Predictive Control Toolbox*, The MathWorks, Inc., Natick, MA (1994).

ABSTRACTS OF PUBLICATIONS

1. Significance Regression: Robust Regression for Collinear Data

Tyler R. Holcomb and Manfred Morari
Chemical Engineering 210-41
California Institute of Technology
Pasadena, CA 91125

Keywords: significance regression, biased regression, PLS, multivariable regression, robust regression, collinearity

Abstract
This paper examines robust linear multivariable regression from collinear data. A brief review of M-estimators discusses the strengths of this approach for tolerating outliers and/or perturbations in the error distributions. The review reveals that M-estimation may be unreliable if the data exhibit collinearity. Next, significance regression (SR) is discussed. SR is a successful method for treating collinearity but is not robust. A new significance regression algorithm for the weighted-least-squares error criterion (SR- WLS) is developed. Using the weights computed via M-estimation with the SR-WLS algorithm yields an effective method that robustly mollifies collinearity problems. Numerical examples illustrate the main points.

2. Significance Regression: A Statistical Approach to Biased Linear Regression and Partial Least Squares

Tyler R. Holcomb, Hakan Hjalmarsson and Manfred Morari
Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena CA, 91125

Keywords: biased regression, PLS, multivariable regression, significance regression, collinearity

Abstract
This paper first examines the properties of biased regressors that proceed by restricting the search for the optimal regressor to a subspace. These properties suggest features such biased regression methods should incorporate. Motivated by these observations, this work proposes a new formulation for biased regression derived from the principle of statistical significance. This new formulation, significance regression (SR), leads to partial least squares (PLS) under certain model assumptions and to more general methods under various other model assumptions. For models with multiple outputs, SR will be shown to have certain advantages over PLS. Using the new formulation a significance test is advanced for determining the number of directions to be used; for PLS, cross- validation has been the primary method for determining this quantity. The prediction and estimation properties of SR are discussed. A brief numerical example illustrates the relationship between SR and PLS.

3. PLS Leads to Different Algorithms for Factor Analysis and Regression

Tyler R. Holcomb and Manfred Morari
Chemical Engineering 210-41
California Institute of Technology
Pasadena, CA 91125

Keywords: biased regression, PLS, multivariable regression, factor analysis, collinearity

Abstract
Two multivariable problems of general interest are factor analysis and regression. This paper examines partial least squares (PLS) as a tool for both problems. For single output data sets, the familiar PLS algorithm is applicable to both problems. For multiple output problems the familiar PLS algorithm (called fact-PLS in this paper) is appropriate for factor analysis. However fact-PLS leads to algebraically-inconsistent results for regression problems. To address this issue, a new algebraically-consistent multivariable PLS algorithm, C-PLS, is developed. Unlike fact-PLS, C-PLS does not rely on iterative calculations. Another PLS approach, "one-at-a-time" PLS (OAT-PLS), is closely related to C-PLS; however OAT-PLS is also algebraically-inconsistent. A simulation study of these various PLS methods shows C-PLS to have the best estimation and prediction performance.

4. Significance Regression: Improved Estimation from Collinear Data for the Measurement Error Model

Tyler R. Holcomb and Manfred Morari
Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena, CA 91125

Keywords: measurement error models, biased regression, partial least squares, multivariable regression, significance regression, collinearity

Abstract
This paper examines improved regression methods for the linear multivariable measurement error model (MEM) when the data suffers from "collinearity." The difficulty collinearity presents for reliable estimation is discussed and a systematic procedure, significance regression (SR-MEM), is developed to address collinearity. In addition to mitigating collinearity difficulties SR-MEM produces asymptotically unbiased estimates. The use of ordinary least squares (OLS) for the MEM is examined. For collinear data OLS can improve the mean squared error of estimation over the maximum likelihood (ML) unbiased estimator in a manner analogous to ridge regression (RR). The significance regression method developed for the classical model (SR- classical) can also be used for data with measurement errors. SR-classical is similar SR- MEM and can yield better estimation than the ML estimator for collinear data. Numerical examples illustrate several points.

5. Identification of Uncertainty Bounds for Robust Control with Applications to a Fixed Bed Reactor

C. Webb, H. Budman and M. Morari*
*Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
A new methodology for computing frequency domain uncertainty bounds for single-input single-output systems is presented. This new methodology uses spectral analysis to identify a series of non-parametric frequency domain models and a "regions-mapping" technique to bound these models in the complex plane. The methodology is compared to existing non-parametric techniques and shown to be superior for identifying the uncertainty bound associated with a nonlinear system. It is applied to the identification of a fixed bed reactor. A robust controller with a single adjustable parameter is designed for the reactor using Internal Model Control (IMC) theory. The computed uncertainty bounds are experimentally validated using the IMC controller.

6. Robust Stability of Constrained Model Predictive Control

A. Zheng and M. Morari
Chemical Engineering 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
A new design technique for a robust model predictive controller is proposed using an uncertainty description expressed in the time-domain. Robust stability of the resulting closed-loop system is guaranteed for a set of Finite Impulse Response (FIR) models. Both necessary and sufficient conditions for asymptotic stability are stated. If the uncertainty is described as lower and upper bounds on impulse response coefficients, then the resulting optimization problem can be cast as a linear program of moderate size.

7. Robust Stability of Linear Systems with Constraints

A. Zheng and M. Morari
Chemical Engineering 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
Despite a rich and complete theory developed for robust control of linear systems, *little* work has been done for robust control of linear systems with *constraints*. In this paper, a synthesis method to design a model predictive controller which optimizes robust performance is proposed for a stable linear time-varying discrete-time system represented by a Finite Impulse Response model. In the absence of constraints, we show that with this method robust Bounded-Input Bounded-Output stability of the resulting closed-loop system is guaranteed. Both necessary and sufficient conditions for robust global asymptotic stability, i.e. offset free tracking for all plants in the set, are stated. Furthermore, robust global asymptotic stability if preserved for a class of asymptotic constant disturbances entering at the plant output.

These results hold for any uncertainty description expressed in the time-domain. However, there is a trade-off between the generality of the uncertainty description and the computational complexity of the resulting optimization problem. For a broad class of uncertainty descriptions, we show that the optimization problem can be cast as a linear program of moderate size.

8. Stability and Robustness Properties of Model Predictive Control of Nonlinear Systems

S.L. de Oliveira and M. Morari
Chemical Engineering 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
In this paper a technique for the design of a robustly stabilizing model predictive controller (MPC) for continuous time-varying nonlinear constrained systems which is easily implementable and computationally inexpensive is introduced. The model used in the calculations is a family of local first order approximations of the dynamics of the plant which makes it possible for the optimization problem to be posed as a convex problem.

The model predictive controller is implemented in a moving horizon fashion where a sequence of optimal control moves for the model is calculated but only the first element of the sequence is actually implemented. Then the states of the plant are either measured (state feedback case) or estimated (output feedback case) and the optimal control calculations are repeated. This procedure is performed until one sampling interval before the end of the horizon of the first optimization problem. Then the next calculated optimal control moves are implemented for the period of a whole prediction horizon and a new sequence of optimal control problems initiates.

This novel "mixed" control strategy is shown to produce less conservative results than a previous version of the algorithm where the measurements were taken only at the end of horizons.

Stability of the closed-loop strategy is shown to produce less conservative results than a previous version of the algorithm where the measurements were taken only at the end of horizons.

The stability constraint does not introduce non-convexities in the optimization problem as will be seen later. Moreover, a somewhat conservative version of this constraint allows the optimization problem to be posed as a simple quadratic programming (QP) problem.

In the state feedback case, the resulting control algorithm is asymptotically stable under certain assumptions on the dynamics of the plant and it is able to handle bounded time-varying disturbances, time-varying parameter deviations from their nominal values and measurement bias.

In the output feedback case, satisfaction of certain conditions on the nonlinear structure of the plant, parameters, disturbances, measurement bias and state estimation errors makes it possible for the combination of a robust asymptotically stable nonlinear controller and observer to result in robust asymptotic stability of the closed-loop system.

Since the nonlinear structure of the dynamics of the plant does not need to be exactly known (as long as it satisfies certain assumptions), the proposed control algorithm is robustly stabilizing with respect to both parametric and structural mismatches between the plant and the family of linear models used for computation of the optimal control law. Even in the output feedback case, modeling errors and unknown time-varying parameters are allowed, i.e., both the controller and the observer are robust.

9. Some Control Problems in the Process Industries

M. Morari
Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
The two problems discussed in this paper, the control of systems with constraints and statistical quality control, have in common that they have attracted much of the academic and industrial interest in the last decade. The problem formulations are motivated, progress toward a solution is summarized, and outstanding issues are indicated.

10. Current Directions in Process Control Theory

M. Morari
Control and Dynamical Systems 210-41
California Institute of Technology
Pasadena, CA 91125

Abstract
Current process control research is focused on issues of identification, in particular "control relevant identification"; the control of nonlinear systems, in particular geometric techniques and model predictive control; and monitoring, diagnostics and quality control. The main ideas in these areas are reviewed and a detailed summary of recent results on the control of linear systems with constraints is presented.