

Structural Design for On-Line Process Optimization: I. Dynamic Economics of MPC

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The structural design of integrated online process optimization and regulatory control systems based on an economic analysis of different structures is addressed. The regulatory control layer is assumed to be implemented using model predictive control (MPC) techniques. An approach to the analysis of the dynamic economics of MPC is presented which uses the state-space formulation as the plant model. Output feedback is performed in the framework of linear quadratic filtering theory using a Kalman filter. Using the unconstrained model predictive control law, the variance of the constrained variables of the closed-loop system subject to stochastic disturbances is analyzed. Based on the variance of the constrained variables, the amount of necessary backoff from the constraints due to regulatory disturbances is calculated and the dynamic economics are established. The dynamic economics of the model predictive regulatory control system are incorporated into the method of the average deviation from optimum analyzing the economic performance of an online optimization system. Thus, different structures of the integrated system of online optimization and MPC-based regulatory control can be analyzed in terms of their economic performance, and the necessary structural design decisions can be taken.

Introduction

A chemical process is usually subject to parametric uncertainty and disturbances which affect the optimum process operating point. One approach to handling these uncertainties and disturbances and to tracking the changing process optimum is model-based real-time optimization. The location of an on-line optimization system in the overall optimal control hierarchy is shown in Figure 1. The process is subject to disturbances over a wide range of frequency. Fast or regulatory disturbances have faster dynamic characteristics than the process and have therefore vanished or changed before the long-term process optimum can change. They are rejected by the regulatory control system which regulates the process at a given operating point. Slowly varying disturbances, on the other hand, change the plant optimum with time (Morari et al., 1980). Examples of slowly varying disturbances are slow time variations and uncertainties in the process parameters such as heat-transfer coefficients, catalyst activities, and quality of the feed flows and changes in market conditions such

as raw material and product prices, availabilities, and demands. In order to track the optimum as it changes with time, process measurements are taken and passed to the on-line optimization system where they are compared to the outputs of a process model. Based on the prediction error, a set of model parameters is estimated. The updated process model is optimized with respect to the regulatory control set points, and the new optimal set points are passed to the regulatory control system, which drives the process to the new optimum operating point. The procedure is repeated after a certain time interval. As described by several authors (Darby and White, 1988; Jiang et al., 1987), this decomposition of the control tasks is industrial practice with even more levels above the optimization layer for the long-term planning and scheduling of plant operation, which will not be considered here. The regulatory control level is assumed to be implemented using model predictive control (MPC) techniques. The application of an integrated MPC and on-line optimization system to an olefins plant and the resulting economic benefits are described by Emoto et al. (1994).

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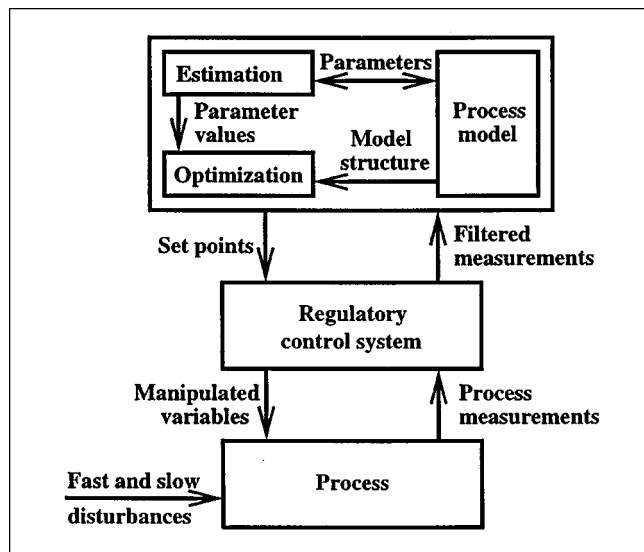


Figure 1. General structure of an on-line optimization system.

The economic benefit of on-line optimization depends on the structure of the on-line optimization system (de Hennin et al., 1994). This structure is determined by the process model used for optimization, the structure of the regulatory control system with its measured and manipulated variables, the process measurements taken for estimating model parameters, the parameters estimated in the model, and the estimation and optimization algorithms with their interactions. de Hennin et al. (1994) and Loeblein and Perkins (1996) addressed the problem of structural design of the online optimization system using the method of the average deviation from optimum. This method estimates the likely economic performance of a given structure of the on-line optimizer. Based on the analysis results for different structures, the on-line optimizer structure with the best economic performance can be selected for implementation.

The method of the average deviation from optimum analyzes the on-line optimizer performance based on the assumption that a perfect regulatory control system is in place, that is, fast, regulatory disturbances are neglected and the process follows set point changes immediately and without offset. The regulatory control layer, which holds the plant as close as possible to the optimal steady state determined by the optimizer, plays a key role in the overall economic performance of the system. Thus, ideally, structural decisions associated with the implementation of this layer should be made with a view to maximizing the potential economic performance of the overall system. The purpose of this two-part article is to relax the assumption of perfect control and analyze the economic performance of an integrated on-line optimization and regulatory control system, in order to take the appropriate structural decisions during the design of an online optimizer.

The dynamic economic performance of the regulatory control system is evaluated by analyzing the dynamic economics of a given control structure. Narraway et al. (1991) define the dynamic economics as the effect of the process dynamics on

the process economics. The basic idea of dynamic economics is shown in Figure 2. The shaded area represents the dynamic region around the steady-state operating point. This region is described by the response of the closed-loop system of process and regulatory control system to the possible disturbances entering the system. The shape and size of the dynamic region is dependent on the process design and the regulatory control structure in terms of manipulated and measured variables, as well as the control algorithms employed. The steady-state operating point should be chosen such that, on the one hand, all points in the dynamic region are feasible with respect to the constraints and, on the other hand, the steady-state operating point is as close as possible to the steady-state optimum. This implies that the structure of the control system together with the controller and its tuning parameters should be chosen such that the amount of constraint backoff is minimized. Based on the idea of dynamic economics, Narraway et al. (1991) and Heath et al. (1996) developed hybrid mixed integer linear programming (MILP) regulatory control structure selection algorithms.

In this work, the regulatory control layer will be assumed to be implemented using linear model predictive control algorithms. There exist large amounts of literature on the different formulations and versions of model predictive control algorithms dealing with issues such as stability and feasibility in the presence of constraints. In order to categorize the developments, a number of review articles have been published, for example, Garcia et al. (1989), Ricker (1991), Rawlings et al. (1994), Lee (1996), and Qin and Badgwell (1996) on industrial MPC technology and, most recently, Morari and Lee (1997).

This article presents an approach to the analysis of the dynamic economics of model predictive control (MPC). The model predictive controller considered uses the state-space formulation as the plant model. Output feedback is performed in the framework of linear quadratic filtering theory using a Kalman filter. The unconstrained model predictive

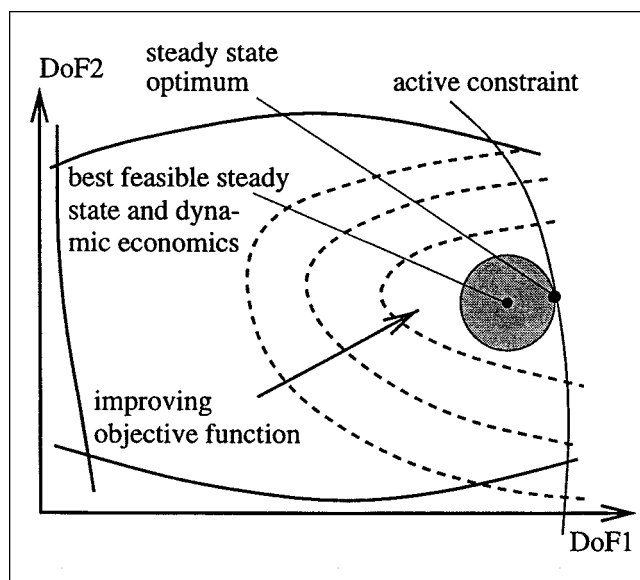


Figure 2. Dynamic economics of process control.

control law is considered. Thus, a closed form solution of the control law can be derived and the variance of the constrained outputs of the closed-loop system subject to stochastic disturbances can be analyzed. Based on the variances of the constrained variables, the amount of necessary backoff from the constraints due to regulatory disturbances is calculated and the dynamic economics are established. The method analyzing the dynamic economics of the model predictive regulatory control layer is then integrated with the established method for the analysis of the likely economic benefit of implementing an on-line optimizer on a plant (de Hennin et al., 1994; Loeblein and Perkins, 1996) which gives a unified measure of the economic performance of the integrated on-line optimization and regulatory control system. The theory is demonstrated in the second part of this article using a simulated fluid-catalytic cracker (FCC) case study.

The dynamic economics are determined for a given structure of the regulatory control system, that is, the set of measured and manipulated variables is fixed as well as the set of tuning parameters. The method does not therefore include a design feature which automatically returns the structure including tuning parameters which gives the best dynamic economics. Similar to the method of the average deviation from optimum, different structures can be examined, which results in a ranking of the considered structures. If the designer of the on-line optimizer has the freedom to design the structure of the regulatory control system as well, the structure of the integrated online optimization and regulatory control system with the best economic performance can be chosen. If the regulatory control structure is fixed, its economic performance is incorporated into the method of the average deviation from optimum and the structure of the on-line optimizer can be chosen such that the combined system of an on-line optimizer and regulatory controller gives the optimal performance.

The model predictive controller formulation used for this work is presented. The dynamic economics of the model predictive control layer are determined using the unconstrained MPC control law, followed by a brief introduction to the method of the average deviation from optimum analyzing the economic performance of different structures of the on-line optimization layer. The analysis method of the MPC regulatory control layer is incorporated into the method of the average deviation from optimum to give a unified measure of performance of the integrated on-line optimization and regulatory control system, followed by a short discussion of the presented theory.

In the second part of this article, the theory is applied to a realistic case study on the optimization and regulatory control of a FCC unit.

Model Predictive Controller Formulation

The model predictive controller considered in the following is based on the formulation presented by Muske and Rawlings (1993). They developed a model predictive controller that uses a linear time-invariant (LTI) state-space model of the process. Output feedback is performed in the framework of linear quadratic filtering theory using a Kalman filter. This section gives a brief introduction to the controller formulation.

The underlying system for the combined observer/regulator is a discrete dynamic LTI model of the process with normally distributed stochastic inputs

$$x(k+1) = Ax(k) + B_u u(k) + B_v v(k) \quad (1)$$

$$y(k) = Cx(k) + D_u u(k) + D_v v(k) + w(k),$$

with

$x(k)$ = state variables
 $u(k)$ = manipulated input variables
 $y(k)$ = output variables
 $v(k)$ = unmeasured disturbance variables
 $w(k)$ = measurement error

The vectors of stochastic variables $v(k)$ representing the fast, stationary process disturbances and $w(k)$ representing the measurement noise are assumed to be Gaussian white noise processes with covariance matrices V and W , respectively. The elements of the vectors $v(k)$ and $w(k)$ are independent so that the covariance matrices V and W are diagonal matrices with zeros off the main diagonal. Typical disturbances in a chemical plant can be modeled in this framework using a linear differential equation driven by white noise v from which the disturbance variable d is determined (Morari and Stephanopoulos, 1980)

$$d(k+1) = \epsilon d(k) + v(k). \quad (2)$$

By keeping ϵ strictly below one, $\epsilon < 1$, the fast and non-persistent, stationary nature of the disturbance can be retained. The linear model of the process is then given by the linear system (Eq. 1) augmented with Eq. 2.

The model predictive controller formulation used in the following is described in detail in Muske and Rawlings (1993). In summary, the algorithm for the calculation of the control moves at time k consists of the following steps:

(1) With $u(k-1)$ applied to the process, and state estimates of the augmented system $\hat{x}(k|k-1)$ and $\hat{p}(k|k-1)$ known, obtain process measurement $y(k)$.

(2) Calculate step disturbance estimate $\hat{p}(k+1|k)$ from the estimation equation of the augmented system (Muske and Rawlings, 1993)

$$\begin{aligned} \hat{p}(k+1|k) &= \hat{p}(k|k-1) \\ &+ L_p [y(k) - C\hat{x}(k|k-1) - D_p \hat{p}(k|k-1) - D_u u(k-1)]. \end{aligned}$$

(3) Calculate new steady-state target values $u_s(k)$ and $x_s(k)$ from the following quadratic program (Muske and Rawlings, 1993)

$$\begin{aligned} \min_{x_s, u_s} \quad & (u_s - \bar{u})^T R_s (u_s - \bar{u}) \\ \text{s.t.} \quad & \begin{bmatrix} I - A & -B_u \\ C & D_u \end{bmatrix} \begin{bmatrix} x_s \\ u_s \end{bmatrix} = \begin{bmatrix} 0 \\ y_t - D_p \hat{p} \end{bmatrix} \\ & u_{\min} \leq u_s \leq u_{\max}. \end{aligned} \quad (3)$$

(4) Calculate the new control moves $u(k)$ by minimizing the controller objective function shown below subject to con-

straints with new steady-state target values $u_s(k)$ and $x_s(k)$ and current estimation error $\omega(k)$ (Muske and Rawlings, 1993)

$$\min_{u^N} (u^N - u_s^N)^T H (u^N - u_s^N) + 2(u^N - u_s^N)^T \times [G(\hat{x}(k|k-1) - x_s) - F(u(k-1) - u_s) + J\omega(k)]. \quad (4)$$

The matrices F , G , H , and J depend on the system matrices, the objective function weighting matrices, and the Kalman filter gain matrices. Their exact definitions are given in the Appendix.

(5) Calculate state estimates $\hat{x}(k+1|k)$ from the estimation equation of the augmented system using the current control moves $u(k)$

$$\hat{x}(k+1|k) = A\hat{x}(k|k-1) + B_u u(k) + L_x [y(k) - C\hat{x}(k|k-1) - D_p \hat{p}(k|k-1) - D_u u(k-1)].$$

(6) Start procedure again from step 1 at the next sampling time $k+1$.

In the next section, the calculation of the regulatory backoff and the dynamic economics of a model predictive control system based on the controller formulation outlined above is presented.

Unconstrained Model Predictive Control

In order to use the advantages of an analytical solution of the control law during the analysis of the dynamic economics of the model predictive controller, the quadratic programming (QP) problem of the MPC control law is considered in the following neglecting input and output constraints. The effect of the disturbances on the outputs is mapped through the closed-loop system using the unconstrained MPC control law. Thus, the variance of the input and output variables to which constraints are to be applied can be determined. From this variance, the amount of backoff from the constraints which guarantees the feasible operation of the process for a given probability and the corresponding dynamic economics of the model predictive controller can be determined.

The calculation of the constraint backoff using the unconstrained model predictive control law is particularly advantageous when analyzing nonminimum phase (NMP) systems. The controller does not attempt to invert the transfer function of the nonminimum phase system in order to meet the constraints and the closed-loop system is not prone to instability due to the (in the case of discrete-time systems) transmission zero outside the unit disk of the NMP system. Instead, the regulatory backoff is calculated from the variation of the constrained variables under closed loop using the unconstrained control law.

Analytical solution of the control law

Since in the following, the unconstrained model predictive control law is considered, the input moves predicted by the controller are determined from the minimization of the con-

troller objective function neglecting input and output constraints

$$\min_{u^N} (u^N - u_s^N)^T H (u^N - u_s^N) + 2(u^N - u_s^N)^T \times [G(\hat{x}(k|k-1) - x_s) - F(u(k-1) - u_s) + J\omega(k)]. \quad (5)$$

This represents an unconstrained quadratic program (QP) which can be solved analytically. Setting the first derivative of the objective function to zero, the optimal value of the N future control moves is obtained, linearly dependent on the current state estimates, the inputs previously applied to the process, and the present estimation error

$$(u^N)^* = u_s^N - H^{-1}G(\hat{x}(k|k-1) - x_s) + H^{-1}F(u(k-1) - u_s) - H^{-1}J\omega(k). \quad (6)$$

Since only the first part of the N future control moves is applied to the process, the first rows of the matrices $H^{-1}G$, $-H^{-1}F$, and $H^{-1}J$ are taken according to the number of manipulated variables n_u

$$\begin{aligned} K_x &= [(H^{-1}G)(i, j)]_{i=1, \dots, n_u; j=1, \dots, n_x} \\ K_u &= [(-H^{-1}F)(i, j)]_{i=1, \dots, n_u; j=1, \dots, n_u} \\ K_\omega &= [(H^{-1}J)(i, j)]_{i=1, \dots, n_u; j=1, \dots, n_y} \end{aligned} \quad (7)$$

The variable n_x represents the number of state variables and n_y is the number of output variables, which is equal to the length of the vector of the estimation error $\omega(k)$. The result is an expression for the input vector at time k with the constant gain matrices K_x , K_u , and K_ω

$$u(k) = u_s - K_x [\hat{x}(k|k-1) - x_s] - K_u [u(k-1) - u_s] - K_\omega \omega(k). \quad (8)$$

Calculation of regulatory backoff

The necessary backoff from the constraints is determined in the following by considering the unconstrained MPC law. Based on the performance of the unconstrained closed-loop system, an operating point is determined which accommodates the fast disturbances without violating the constraints.

The closed-loop system of the process with the combined observer/regulator applied is shown in Figure 3. It is assumed that the behavior of the process can be represented by the linear time-invariant system shown below

$$\begin{aligned} x(k+1) &= Ax(k) + B_u u(k) + B_v v(k) \\ y(k) &= Cx(k) + D_u u(k) + D_v v(k). \end{aligned} \quad (9)$$

The transfer function blocks of the Kalman filter and the model predictive controller both represent linear relationships between their input and output variables. Thus, it is possible to represent the closed-loop system as one linear

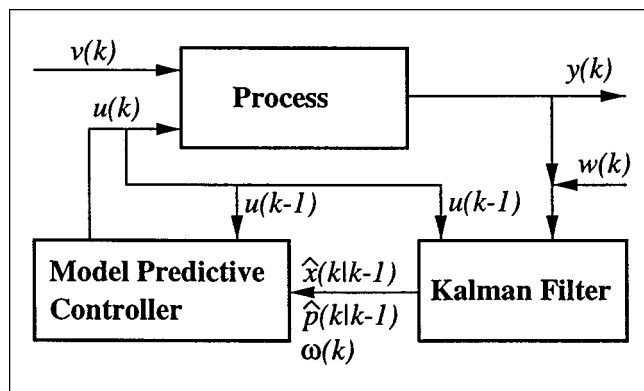


Figure 3. Closed-loop system.

time-invariant (LTI) state-space system of higher order with the stochastic disturbances and the measurement noise as inputs (see Figure 4). The behavior of LTI systems can be analyzed easily so that the stochastic disturbances and measurement noise can be mapped through the closed-loop system and their effect on the constrained input and output variables determined. Both the disturbances and the measurement noise are assumed to be Gaussian white noise processes with known covariances. Since the closed-loop system is represented by an LTI state-space system as shown in Figure 4, the covariance of the constrained inputs and outputs can be determined and the necessary backoff from the constraints can be calculated.

The LTI state-space formulation of the closed-loop system is derived from the following equations which represent the linear relationships of each of the transfer function blocks in Figure 3. The derivation is along the lines of the controller algorithm given in the previous section.

(1) The process with its state and output variables is described by the following LTI state-space system

$$x(k+1) = Ax(k) + B_u u(k) + B_v v(k) \quad (10)$$

$$y(k) = Cx(k) + D_u u(k) + D_v v(k).$$

(2) The Kalman filter calculates the estimates of the process states $\hat{x}(k+1|k)$ and the output step disturbances $\hat{p}(k+1|k)$ from the measurements of the system

$$\begin{aligned} \hat{x}(k+1|k) &= A\hat{x}(k|k-1) + B_u u(k) \\ &+ L_x [y(k) - C\hat{x}(k|k-1) - D_p \hat{p}(k|k-1) - D_u u(k-1)] \end{aligned} \quad (11)$$

$$\begin{aligned} \hat{p}(k+1|k) &= \hat{p}(k|k-1) \\ &+ L_p [y(k) - C\hat{x}(k|k-1) - D_p \hat{p}(k|k-1) - D_u u(k-1)]. \end{aligned} \quad (12)$$

The relationship for the process measurements including measurement noise is given below

$$y(k) = Cx(k) + D_u u(k-1) + D_v v(k) + w(k). \quad (13)$$

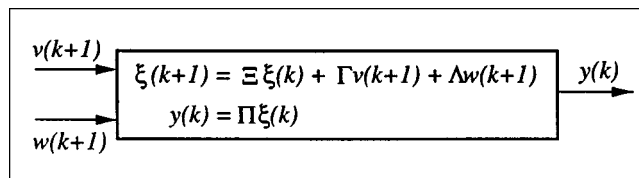


Figure 4. State-space representation of the closed-loop system.

(3) The next step is the calculation of the new steady-state target values $u_s(k)$ and $x_s(k)$, which remove the output step disturbance at steady state. As described above, they are determined from the solution of the quadratic program (Eq. 3) (Muske and Rawlings, 1993). However, assuming that the control system is square, that is, the number of controlled variables is equal to the number of manipulated variables, the solution is entirely determined by the equality constraints representing the system equations

$$\begin{bmatrix} I - A & -B_u \\ C & D_u \end{bmatrix} \begin{bmatrix} x_s \\ u_s \end{bmatrix} = \begin{bmatrix} 0 \\ y_t - D_p \hat{p} \end{bmatrix}. \quad (14)$$

In this case, there are no degrees of freedom to minimize the least-squares objective function and the steady-state target values are obtained directly from the linear system equations

$$u_s(k) = -[C(I - A)^{-1}B_u + D_u]^{-1}D_p \hat{p}(k+1|k) \quad (15)$$

$$\begin{aligned} x_s(k) &= -(I - A)^{-1}B_u[C(I - A)^{-1}B_u + D_u]^{-1} \\ &\times D_p \hat{p}(k+1|k). \end{aligned} \quad (16)$$

The output target values y_t are zero since the analysis is carried out at the nonlinear optimum, where the system was linearized.

If the system is not square, similar analytical expressions for the input and state target values can be obtained. The quadratic program (Eq. 3) can be solved analytically since the inequality constraints on the input variables are neglected during the backoff calculation. Without the input inequality constraints, only equality constraints from the linear system equations are present and the QPs can be solved analytically in the reduced space.

(4) The last step is the calculation of the control moves from the solution of the unconstrained model predictive control law. The following expression for the manipulated variables at time k is obtained, linearly dependent on the state estimates $\hat{x}(k|k-1)$, the estimation error $\omega(k)$, the previous input variables $u(k-1)$, and the steady-state target values $u_s(k)$ and $x_s(k)$

$$\begin{aligned} u(k) &= u_s(k) - K_x [\hat{x}(k|k-1) - x_s(k)] \\ &- K_u [u(k-1) - u_s(k)] - K_\omega \omega(k). \end{aligned} \quad (17)$$

The estimation error $\omega(k)$ is given by the difference between

the process measurements and the model outputs

$$\omega(k) = y(k) - C\hat{x}(k|k-1) - D_p\hat{p}(k|k-1) - D_u u(k-1). \quad (18)$$

With straightforward, but extensive, algebraic manipulations, Eqs. 10–18 can be rearranged to eliminate $u_s(k)$ and $x_s(k)$ and write the system in the form of a linear discrete-time state-space model of the closed-loop system

$$\begin{bmatrix} x(k+1) \\ \hat{x}(k+1|k) \\ u(k+1) \\ \hat{p}(k+1|k) \end{bmatrix} = \begin{bmatrix} A & 0 & B_u & 0 \\ L_x C & A - L_x C & B_u & -L_x D_p \\ Z_1 & Z_2 & Z_3 & Z_4 \\ L_p C & -L_p C & 0 & (I - L_p D_p) \end{bmatrix} \begin{bmatrix} x(k) \\ \hat{x}(k|k-1) \\ u(k) \\ \hat{p}(k|k-1) \end{bmatrix} + \begin{bmatrix} B_v \\ L_x D_v \\ Z_5 \\ L_p D_v \end{bmatrix} v(k) + \begin{bmatrix} 0 \\ 0 \\ Z_6 \\ 0 \end{bmatrix} v(k+1) + \begin{bmatrix} 0 \\ L_x \\ Z_7 \\ L_p \end{bmatrix} w(k) + \begin{bmatrix} 0 \\ 0 \\ Z_8 \\ 0 \end{bmatrix} w(k+1). \quad (19)$$

The matrices Z_i stand for lengthy matrix expressions containing matrices from Eqs. 10–18. Their definitions are given in the Appendix. In order to analyze the performance of the closed-loop system, the system in Eq. 19 needs to be reformulated such that the explicit dependence of the righthand side on both $v(k)$ and $v(k+1)$ (and similarly on $w(k)$ and $w(k+1)$) is removed. This is achieved by augmenting the state vector with $v(k)$ and $w(k)$. The result is a linear time-invariant state-space model of the closed-loop system with the normally distributed disturbances $v(k+1)$ and measurement noise $w(k+1)$ as input variables

$$\xi(k+1) = \Xi \xi(k) + \Gamma v(k+1) + \Lambda w(k+1) \quad (20)$$

$$y(k) = \Pi \xi(k).$$

The state vector $\xi(k)$ consists of the following variables

$$\xi(k)$$

$$= \begin{bmatrix} x(k)^T & \hat{x}(k|k-1)^T & u(k)^T & \hat{p}(k|k-1)^T & v(k)^T & w(k)^T \end{bmatrix}^T. \quad (21)$$

The exact definitions of the matrices Ξ , Γ , Λ , and Π are given in the Appendix.

Having obtained the closed-loop system in the form of the linear state-space model in Eq. 20, the evolution of the state vector $\xi(k)$ over time can be determined. The model of the closed-loop system in Eq. 20 represents a linear state-space model driven by Gaussian white noise. Since the closed-loop system is linear, the state and output variables $\xi(k)$ and $y(k)$ are also normally distributed and the covariances of $\xi(k)$ and $y(k)$ can be determined as functions of the covariances of the disturbances $v(k)$ and measurement noise $w(k)$. The evolution of the state vector $\xi(k)$ over time is given by the following predictor equation

$$\xi(k) = \Xi^k \xi(0) + \sum_{j=0}^{k-1} \Xi^j \Gamma v(k-j) + \sum_{j=0}^{k-1} \Xi^j \Lambda w(k-j). \quad (22)$$

The variable $\xi(0)$ represents the initial state of the system. Since the variables $\xi(k)$, $v(k+1)$ and $w(k+1)$ are all uncorrelated, the covariance of the state vector of the closed-loop system can be determined as a function of the covariances of the disturbances V , the measurement noise W , and the initial state Σ

$$\begin{aligned} \text{cov}[\xi(k)] &= \Xi^k \Sigma (\Xi^k)^T \\ &+ \sum_{j=0}^{k-1} \Xi^j \Gamma V \Gamma^T (\Xi^j)^T + \sum_{j=0}^{k-1} \Xi^j \Lambda W \Lambda^T (\Xi^j)^T. \end{aligned} \quad (23)$$

Since the closed-loop system with a stable process and a stable observer/regulator (which follows in the unconstrained case from the separation principle) is also stable, the covariance of the states for $k \rightarrow \infty$ is then given by

$$\text{cov}(\xi) = \Delta + \Omega. \quad (24)$$

The matrices Δ and Ω are the solutions of the discrete Lyapunov equations as those equations determine the values of the infinite sums in Eq. 23 for $k \rightarrow \infty$

$$\Delta = \Gamma V \Gamma^T + \Xi \Delta \Xi^T \quad (25)$$

$$\Omega = \Lambda W \Lambda^T + \Xi \Omega \Xi^T.$$

The covariance of the input variables may be determined from $\text{cov}(\xi)$, since the state vector of the closed-loop system ξ contains the manipulated variables of the process $u(k)$. The covariance of the process output variables $y(k)$ can be obtained from the covariance of the state variables

$$\text{cov}(y) = \Pi \text{cov}(\xi) \Pi^T = \Pi (\Delta + \Omega) \Pi^T \stackrel{\text{def}}{=} \Psi. \quad (26)$$

Having obtained the covariance matrix of the variables to which constraints are to be applied, the necessary backoff from the constraints can be determined in the following way. The variance of an individual variable is given by the corresponding diagonal element of Ψ and the statistical variation of the variables to which constraints are to be applied can be described by the density function f of a Gaussian distribution with zero mean and known covariance (Papoulis, 1991)

$$f(y) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{\text{diag}(\Psi)}} \exp\left(-\frac{y^2}{2\text{diag}(\Psi)}\right). \quad (27)$$

If the constraints are formulated in a way that the constrained variable is required to stay below a certain value, say $y \leq y_{\max}$ for output constraints, the vector of regulatory backoffs β_{reg} from each of the constraints is determined such that the variance of the constrained variable y remains below $y_{\max} + \beta_{\text{reg}}$ for a given probability α

$$\begin{aligned} \alpha &= P(y \leq y_{\max} + \beta_{\text{reg}}) \\ &= \int_{-\infty}^{\beta_{\text{reg}} + y_{\max}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{\text{diag}(\Psi)}} \exp\left(-\frac{y^2}{2\text{diag}(\Psi)}\right) dy. \end{aligned} \quad (28)$$

With the definition of the error function

$$\text{erf}\left(\frac{y}{\sqrt{2}}\right) = \sqrt{\frac{2}{\pi}} \int_0^y \exp\left(-\frac{\tau^2}{2}\right) d\tau, \quad (29)$$

the regulatory backoff for not violating an individual constraint with a probability of $\alpha\%$ is given by the equation shown below

$$\beta_{\text{reg}} = -y_{\max} + \sqrt{2} \sqrt{\text{diag}(\Psi)} \text{erf}^{-1}(2\alpha - 1). \quad (30)$$

The probability α for which feasible operation is required is specified *a priori*. It should be noted that there is an $\alpha\%$ probability of not violating each individual constraint, but a smaller probability of not breaking any constraint due to the fact that the constrained variables are not statistically independent. If the resulting backoff is negative, the variation of y stays within the required bounds for the given probability, α without introducing a backoff. In this case, β_{reg} is set to zero. The regulatory backoff from input constraints is determined in a similar way from the covariance of the constrained inputs which is given by the appropriate diagonal elements of the state variable covariance matrix $\text{cov}(\xi) = \Delta + \Omega$.

Steady-state operating point and dynamic economics

The dynamic economics of a process with its regulatory control system are defined as the economics of the best feasible steady-state operating point of the process subject to disturbances (Naraway et al., 1991; Heath et al., 1996). Mathematically, the dynamic economics can be calculated in

two ways (Heath et al., 1996). One option considers the first-order economic impact of the changes in the slack variables of the inequality constraints of the nonlinear system. Since the first-order sensitivity of the objective function to changes in the slack variables of the inequality constraints is given by the Lagrange multipliers, λ in the Karush-Kuhn-Tucker (KKT) optimality conditions, the dynamic economics can be estimated using (Naraway et al., 1991; Heath et al., 1996)

$$\Delta\Phi = \sum_{i=1}^m \lambda_i \beta_i. \quad (31)$$

This approach gives a linear estimate to the dynamic economics of a given structure of the control system under the assumption that there is no change in the active constraint set once the regulatory backoff β is introduced. Although this approach yields an estimate of the dynamic economics, the best feasible steady-state operating point cannot be determined.

Another possibility is the solution of a linear program (LP), which is obtained from a linearization of the nonlinear system at the nominal optimum steady-state operating point (Heath et al., 1996)

$$\begin{aligned} \min_u \quad & \Delta\Phi = ax + bu \\ \text{s.t.} \quad & 0 = Ax + Bu \\ & y = Cx + Du \\ & -\sigma_0 + \beta \leq Ex + Fu \\ & -\sigma_{uh,0} + \beta_u \leq -Iu \\ & -\sigma_{ul,0} + \beta_u \leq Iu \\ & u^{\text{low}} \leq u \leq u^{\text{high}}. \end{aligned} \quad (32)$$

The variables σ_0 denote the slack variables of the inequality constraints at the nominal optimum where the linearization is performed. For active inequality constraints, the corresponding slack variable σ_0 is zero. Since the linearization of the system is performed at the nominal steady-state optimum, the first-order KKT conditions are satisfied. This implies that, without process disturbances ($\beta = 0$), the objective function $\Delta\Phi$ at the solution of the above LP is zero (Heath et al., 1996). For positive constraint backoffs β , the solution of the LP $\Delta\Phi$ gives a linear estimate of the loss in economic performance due to moving the operating point inside the feasible region of the process in order to ensure feasible operation in the presence of disturbances. At the same time, constraint backoffs from inequality constraints, which are not active at the nominal optimum, are considered and possible changes in the active constraint set due to the regulatory backoff are taken into account. Additionally, the best feasible steady-state operating point of the process, y_s , x_s , and u_s , is returned. The steady-state operating point is then moved inside the feasible region accordingly by changing the set points to the controlled output variables. Thus, the feasible operation of the process in the presence of disturbances is guaranteed.

For square, fully constrained systems, the best feasible steady-state operating point can also be determined in a different manner. At steady state, the following relationship holds for the linear discrete-time system

$$\begin{aligned}x_s &= Ax_s + B_u u_s \\ y_s &= Cx_s + D_u u_s.\end{aligned}\quad (33)$$

From this, the input-output relationship shown below can be obtained

$$y_s = [C(I - A)^{-1}B_u + D_u]u_s. \quad (34)$$

If the system is square and fully constrained, the number of constrained input and output variables is equal to the total number of output variables (or input variables). The input and output variables, which are at their active constraints, are set equal to their corresponding backoff value. The result is a system of linear equations from which the steady-state values of the unconstrained input and output variables can be determined.

Introduction to the Method of the Average Deviation from Optimum

Due to different error sources, which are present during on-line optimization, such as measurement errors, modeling errors, and parametric uncertainties, the optimizer will usually not predict the true process optimum. Instead, there will be a deviation from the true optimum and the possible predicted set points will lie somewhere in a blurred region around the true optimum. This can be seen in Figure 5, where the constraint diagram of a process with two degrees of freedom for optimization is shown. Instead of doing extensive simulations to analyze the performance of the on-line optimizer, de Hennin et al. (1994) developed the method of the average

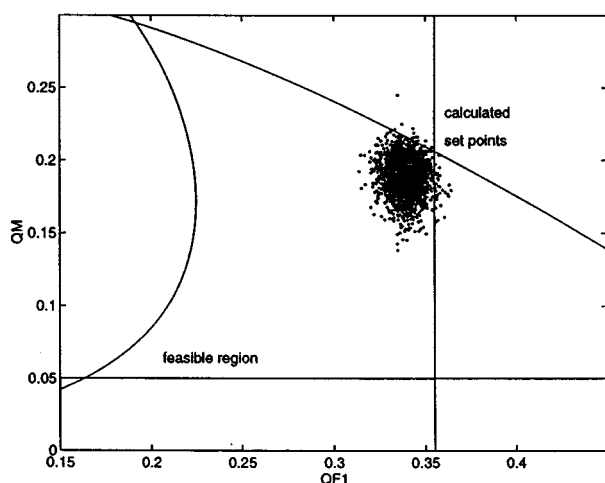


Figure 5. Backoff from active constraints and variation of the predicted set points in the feasible region.

deviation from optimum. This method estimates the likely economic benefit of a given on-line optimizer structure by analyzing how close to the true optimum the process can be operated. de Hennin et al. (1994) neglected the effect of the dynamics of the regulatory control level together with fast (regulatory) disturbances and assumed that the process follows set point changes immediately and without offset. In addition to that, the method was developed for a rigorous optimization model, where the plant-model mismatch consists only in the parameter values. The error sources are described by a normally distributed measurement error ϵ with a given standard deviation σ_ϵ , and a variation in the process parameters. This variation consists of a normally distributed uncertainty η with given standard deviation σ_η and a time variation $\delta\bar{p}(t)$ around a nominal value $\delta p = \eta + \delta\bar{p}(t)$. The method was extended by Loeblein and Perkins (1996) to consider the implementation of approximate optimization models, which feature structural modeling error compared to a rigorous model representing the process. Thus, the structural decisions that can be addressed using the method of the average deviation from optimum are the selection of estimated model parameters, the process variables measured for parameter estimation, and the selection of the optimization model. Additionally, the effect of different set point variables on the steady-state performance of the on-line optimizer may be examined.

The method of the average deviation from optimum is based on an approximation of the nonlinear problem around its nominal optimum. The nominal optimum is determined by minimizing an economic objective function Φ with respect to the set point variables r subject to the nonlinear process model f , and a set of operational feasibility constraints g

$$\begin{aligned}\min_r \quad & \Phi(x, r, p) \\ \text{s.t.} \quad & f(x, r, p) = 0 \\ & g(x, r, p) \leq 0 \\ & y = h(x, r, p).\end{aligned}\quad (35)$$

The parameter vector p is set at the nominal values of the uncertain parameters. The nominal parameter values are those around which the parametric variations and uncertainties are defined. In order to obtain an approximation of the nonlinear model, a second-order Taylor series expansion of the objective function Φ at the nominal optimum is carried out. The set of active constraints at the nominal optimum g and the possible process measurements y are linearized with respect to the set points r and the parameters p to obtain the following first- and second-order perturbation model

$$\begin{aligned}\delta\Phi(\delta r, \delta p) &= C_1\delta r + \delta p^T C_2\delta r + \frac{1}{2}\delta r^T C_3\delta r + C_4\delta p \\ &\quad + \frac{1}{2}\delta p^T C_5\delta p\end{aligned}$$

$$\delta g(\delta r, \delta p) = G\delta p + H\delta r = 0 \quad (36)$$

$$\delta y = J\delta p.$$

If an approximate optimization model including structural plant-model mismatch is used, a first- and second-order perturbation model of this form is obtained from the nonlinear approximate optimization model and the rigorous model representing the process (Loeblein and Perkins, 1996). Due to this approximation of the problem, it is possible to derive analytical expressions for the model parameter estimates $\delta \hat{p}_m$ and the optimal set points predicted by the optimizer $\delta r^*(\delta \hat{p}_m, \beta)$ and map the effects of the different error sources through the parameter estimation and optimization steps. The deviation of the predicted from the true optimum can be determined and averaged over the different error sources. The result is an analytical expression for the average deviation from optimum Θ for a given on-line optimizer structure which is dependent on the backoff β (see below), the covariance of the statistical uncertainty in the parameters σ_η , the covariance of the measurement error σ_ϵ , the structural plant-model mismatch Δy and Δr , and the time variation of the process parameters $\delta \bar{p}(t)$ within the optimization period $t_2 - t_1$

$$\begin{aligned} \Theta &= \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \{ \delta \Phi[\delta r^*(\delta p), \delta p] \\ &\quad - \delta \Phi[\delta r^*(\delta \hat{p}_m, \beta), \delta p] \} f(\eta) f(\epsilon) d\eta d\epsilon dt \\ &= \Theta(\beta, \sigma_\eta, \sigma_\epsilon, \delta \bar{p}(t), t_2 - t_1, \Delta y, \Delta r). \end{aligned} \quad (37)$$

The average deviation from optimum Θ can be calculated for a given on-line optimizer structure and provides an estimate of its economic benefit. The result is a ranking of different on-line optimizer structures in terms of their economic performance. The structure with the best economic performance can be selected for implementation.

In order to ensure the calculation of feasible set points during the optimization, a backoff β from the active constraints is introduced into the optimization step

$$\begin{aligned} \min_{\delta r} \quad & C_1 \delta r + \delta \hat{p}^T C_2 \delta r + \frac{1}{2} \delta r^T C_3 \delta r \quad (38) \\ \text{s.t.} \quad & G \delta r + H \delta \hat{p} + \beta = 0. \end{aligned}$$

The basic idea is shown in Figure 5. The true process optimum usually lies on a boundary of the feasible region defined by one or more active constraints. Due to the uncertainty in the process parameters and the measurement errors, the set points calculated by the optimizer would lie in a blurred region around the process optimum and a high percentage of the set points would be infeasible. By introducing a backoff from the active constraints into the optimization model, the region of possible set points is moved inside the feasible region of the process. This ensures, on the one hand, the feasible operation of the process for a high probability while, on the other hand, still operating the process as closely to the true optimum as possible. The size of the constraint backoff is dependent on the different error sources, namely, the

amount of measurement error and parameter variation including uncertainty.

Integration of the Average Deviation from Optimum and the MPC Dynamic Economics

In this section, the analysis methods for the MPC regulatory control layer (dynamic economics) and the optimization level (average deviation from optimum) are integrated in order to obtain a unified measure for the economic performance of the integrated on-line optimization and regulatory control system. The approach is based on the work of Morari et al. (1980) who proposed to decompose the overall optimal control problem into an optimization task and a regulatory control task. Furthermore, the disturbances are partitioned into stationary and nonstationary disturbances considering the persistence of a disturbance and its expected value over a suitable time horizon. The nonstationary disturbances are also called slowly varying disturbances since their expected value is nonzero over the time interval. They affect the steady-state optimum of the process and cause a slow time variation of the process optimum. Examples include changing external data like energy costs and slow variations or uncertainties in process parameters. Every optimization interval, the on-line optimizer determines a new optimum steady-state operating point with respect to the slowly varying disturbances. On the other hand, the stationary disturbances are fast disturbances which do not change the steady-state optimum since their expected value is essentially zero after a short time. They have vanished before the steady-state optimum of the process can change. However, the fast disturbances affect the size of the dynamic operating region around the optimum steady-state operating point (Narraway et al., 1991). They are rejected by the regulatory control system.

The dynamic economics of a given control structure are defined as the loss of economic performance due to the introduction of the necessary constraint backoffs which try to guarantee the feasible operation of the process in the presence of disturbances (Narraway et al., 1991). The dynamic economics of a given structure of the control system are obtained from the solution of the linear program (LP) (Eq. 32). The LP is obtained from a linearization of the nonlinear system at the nominal optimum steady-state operating point. For positive constraint backoffs β , the solution of the LP, $\Delta \Phi$ gives a linear estimate of the loss in economic performance due to the introduction of some conservatism in the form of the regulatory backoff in order to ensure the feasible operation of the process subject to disturbances.

The analysis methods of the optimization layer (average deviation from optimum) and the regulatory control level (dynamic economics) have different characteristics in two respects. The first and more obvious point is that the dynamic economics are based on a linearization of the objective function at the nominal optimum and provide a linear estimate of the loss in economic performance due to the regulatory backoff. The method of the average deviation from optimum, on the other hand, considers a more accurate approximation of the objective function by using second-order information in the form of a second-order Taylor series expansion of the objective function at the nominal optimum (de Hennin et al.,

$$\min_{\delta r} \delta \Phi = C_1 \delta r + \delta p^T C_2 \delta r + \frac{1}{2} \delta r^T C_3 \delta r + C_4 \delta p + \frac{1}{2} \delta p^T C_5 \delta p$$

$$\text{s.t. } \delta g = G \delta p + H \delta r = 0. \quad (39)$$

Apart from the fact that the second-order approximation is more accurate, it is in particular advantageous for partially constrained problems where the LP (Eq. 32) becomes degenerate. As can be seen in Figure 6, there is a danger in this case of finding a solution to the LP which is at one of the vertices of the feasible region. Although this does not change the dynamic economics $\Delta \Phi$ due to the linearization of the objective function, this solution would not reflect the true optimal operating point u_s , accommodating the regulatory backoff. The second point is the handling of active and inactive constraints. The method of the average deviation from optimum is based on the assumption that the set of active constraints does not change. It is only locally valid around the active constraints and returns just the necessary backoff from the active constraints. As opposed to that, the method of dynamic economics solving LP (Eq. 32) incorporates the necessary backoff from the inactive constraints, as well. If the backoff is bigger than the slack variable at the nominal optimum, the solution of the LP finds an operating point that also ensures feasible operation with respect to the constraints which are inactive at the nominal optimum.

In integrating the two analysis methods for the optimization and regulatory control layers, we shall assume that the backoffs calculated for each layer may be added to give a total constraint backoff β_{tot} , accommodating both slowly varying and fast disturbances

$$\beta_{\text{tot}} = \beta_{\text{opt}} + \beta_{\text{reg}}. \quad (40)$$

The corresponding loss in economic performance is then esti-

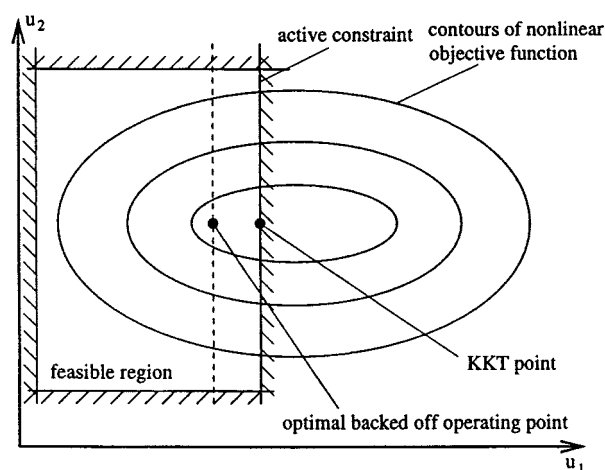


Figure 6. Linear approximation of partially constrained NLP.

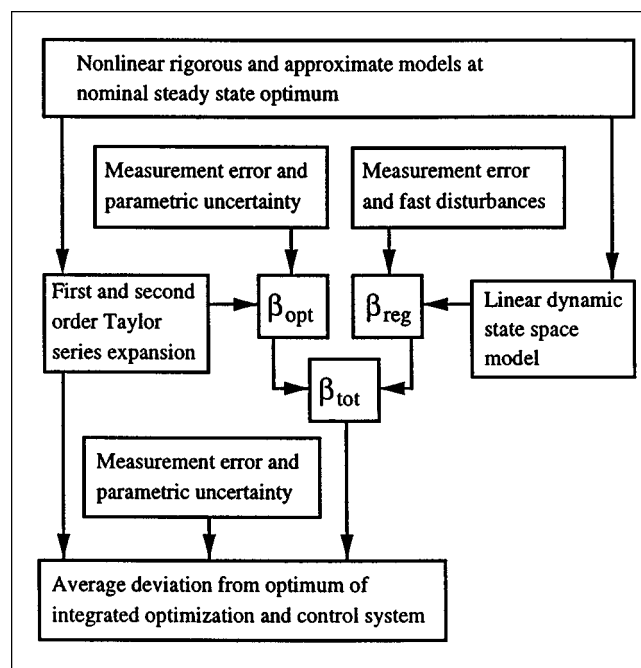


Figure 7. Algorithm for the calculation of the average deviation from optimum.

mated using the second-order approximation of the objective function by introducing the total backoff β_{tot} into the expression calculating the average deviation from optimum for a given on-line optimizer structure (see Eq. 37). Thus, the dynamic economics of the model predictive regulatory control system enter the performance analysis of the integrated system through the total necessary backoff which comprises both the regulatory and optimizing backoff. The result is an analytical expression for the average deviation from optimum of a given structure of an integrated on-line optimization and regulatory control system

$$\Theta = \Theta(\beta_{\text{tot}}, \sigma_{\eta}, \sigma_{\epsilon}, \delta \bar{p}(t), t_2 - t_1, \Delta y, \Delta r). \quad (41)$$

The complete algorithm for the calculation of the average deviation from optimum for the integrated on-line optimization and regulatory control system is summarized in Figure 7.

One issue that has not been addressed in this article is the robust performance of the regulatory control system in the presence of parametric uncertainty and slow disturbances. As Lee (1996) points out, the theory for designing a robust model predictive controller for systems with parametric uncertainty does not seem to be very well established at this point and is still subject to substantial research efforts. Furthermore, a robust MPC formulation is quite likely not to allow an analytical solution of the control law. This implies that it would not be possible to analyze the dynamic economics of the MPC regulatory control layer using an analytical approach. Instead, numerical calculation of the dynamic economics would be required. This would not fit into the analytical method of the average deviation from optimum for the integrated on-line optimization and regulatory control system proposed in this

article. Therefore, robustness issues at the regulatory control level are not addressed in this work.

Conclusions

In this article, the analysis of the dynamic economic performance of the model predictive control layer has been addressed. The approach is based on the solution of the unconstrained model predictive control law. The closed-loop system of controller and process can be formulated as a linear state-space system with disturbances and measurement noise as input variables. Thus, the variance of the constrained variables can be determined and the regulatory constraint backoff can be calculated. The economic analysis methods of the MPC regulatory control layer and the analysis method of the average deviation from optimum for the on-line optimization level (de Hennin et al., 1994; Loeblein and Perkins, 1996) have been integrated. The result is a unified measure of the economic performance of a given structure of an integrated on-line optimization and MPC regulatory control system. Different structures can be compared and the structure with the best economic performance can be chosen for implementation.

Notation

A = linear state-space model matrix
 B = linear state-space model matrix
 C = linear state-space model matrix
 D = linear state-space model matrix
 $\mathbb{E}\{\cdot\}$ = expectation operator
 F = MPC objective function matrix
 G = MPC objective function matrix
 H = MPC objective function matrix
 J = MPC objective function matrix
 k = sample time
 K = gain matrices
 L = Kalman filter gain
 N = input prediction horizon
 P = probability
 Q = output weighting matrix in MPC objective function
 R = input weighting matrix in MPC objective function
 S = control action weighting matrix in MPC objective function
 t = time
 Γ = matrix in state-space representation of closed-loop system
 δ = perturbation variable around nominal optimum
 ϵ = normally distributed measurement error
 Λ = matrix in state-space representation of closed-loop system
 Ξ = matrix in state-space representation of closed-loop system
 Π = matrix in state-space representation of closed-loop system

Subscripts and superscript

s = steady-state value
 t = target value
 $\hat{\cdot}$ = estimate; \hat{p} is an estimate of p

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Appendix: Definition of Matrices

Matrix definitions of the model predictive controller

The unconstrained model predictive control law can be written in the following way

$$\min_{u^N} (u^N)^T H u^N + 2(u^N)^T [G\hat{x}(k|k-1) - Fu(k-1) + J\omega(k)].$$

The objective function matrices are given by

$$F = \begin{bmatrix} S \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$G = \begin{bmatrix} B_u^T \bar{Q} A + D_u^T \bar{Q} C \\ B_u^T \bar{Q} A^2 + D_u^T \bar{Q} C A \\ B_u^T \bar{Q} A^3 + D_u^T \bar{Q} C A^2 \\ \vdots \\ B_u^T \bar{Q} A^N + D_u^T \bar{Q} C A^{N-1} \end{bmatrix}$$

$$J = \begin{bmatrix} D_u^T Q C M + B_u^T \bar{Q} L \\ D_u^T Q C L + B_u^T \bar{Q} A L \\ D_u^T Q C A L + B_u^T \bar{Q} A^2 L \\ \vdots \\ D_u^T Q C A^{N-2} L + B_u^T \bar{Q} A^{N-1} L \end{bmatrix}$$

$$H = \begin{bmatrix} D_u^T Q D_u & 0 & \cdots & 0 \\ 0 & D_u^T Q D_u & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_u^T Q D_u \end{bmatrix}$$

$$+ \begin{bmatrix} 2S + R & -S & 0 & \cdots & 0 \\ -S & 2S + R & -S & \cdots & 0 \\ 0 & -S & 2S + R & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 2S + R \end{bmatrix}$$

$$+ \begin{bmatrix} B_u^T \bar{Q} B_u & B_u^T A^T \bar{Q} B_u & \cdots & B_u^T A^{T^{N-1}} \bar{Q} B_u \\ B_u^T \bar{Q} A B_u & B_u^T \bar{Q} B_u & \cdots & B_u^T A^{T^{N-2}} \bar{Q} B_u \\ \vdots & \vdots & \ddots & \vdots \\ B_u^T \bar{Q} A^{N-1} B_u & B_u^T \bar{Q} A^{N-2} B_u & \cdots & B_u^T \bar{Q} B_u \end{bmatrix}$$

$$+ \begin{bmatrix} 0 & B_u^T C^T Q D_u & \cdots & B_u^T A^{T^{N-2}} C^T Q D_u \\ D_u^T Q C B_u & 0 & \cdots & B_u^T A^{T^{N-3}} C^T Q D_u \\ \vdots & \vdots & \ddots & \vdots \\ D_u^T Q C A^{N-2} B_u & D_u^T Q C A^{N-3} B_u & \cdots & 0 \end{bmatrix}.$$

Matrix definitions of the closed-loop state-space system

Linear discrete-time state-space model of the closed-loop system based on the unconstrained model predictive control law

$$\xi(k+1) = \Xi \xi(k) + \Gamma v(k+1) + \Lambda w(k+1)$$

$$y(k) = \Pi \xi(k).$$

The matrices Ξ , Γ , Λ and Π are defined as follows

$$\Xi = \begin{bmatrix} A & 0 & B_u & 0 & B_v & 0 \\ L_x C & A - L_x C & B_u & -L_x D_p & L_x D_v & L_x \\ Z_1 & Z_2 & Z_3 & Z_4 & Z_5 & Z_7 \\ L_p C & -L_p C & 0 & I - L_p D_p & L_p D_v & L_p \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} 0 \\ 0 \\ Z_6 \\ 0 \\ I \\ 0 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} 0 \\ 0 \\ Z_8 \\ 0 \\ 0 \\ I \end{bmatrix}$$

$$\Pi = [C \ 0 \ D_u \ 0 \ D_v \ 0].$$

The matrices Z_i are given by

$$G_u = [C(I - A)^{-1} B_u + D_u]^{-1} D_p$$

$$G_x = (I - A)^{-1} B_u G_u$$

$$M = K_d + K_x G_x L_p + (I + K_u) G_u L_p$$

$$Z_1 = (-K_x + MC) L_x C$$

$$- [K_x G_x + (I + K_u) G_u - MD_p] L_p C - MCA$$

$$Z_2 = (-K_x + MC)(A - L_x C)$$

$$+ [K_x G_x + (I + K_u) G_u - MD_p] L_p C$$

$$Z_3 = (-K_x + MC) B_u - K_u - MCB_u$$

$$Z_4 = (K_x - MC) L_x D_p$$

$$- [K_x G_x + (I + K_u) G_u - MD_p] (I - L_p D_p)$$

$$Z_5 = (-K_x + MC) L_x D_v$$

$$- [K_x G_x + (I + K_u) G_u - MD_p] L_p D_v - MCB_v$$

$$Z_6 = -MD_v$$

$$Z_7 = (-K_x + MC) L_x - [K_x G_x + (I + K_u) G_u - MD_p] L_p$$

$$Z_8 = -M.$$

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