MODEL PREDICTIVE CONTROL OF A TUBULAR AMMONIA REACTOR-HEAT EXCHANGER SYSTEM WITH SQUARE AND NON-SQUARE CONTROL STRUCTURES USING SINGULAR VALUE DECOMPOSITION (SVD)
Part I: Development of the MPC Algorithm and SVD Computation

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ABSTRACT

This paper presents a multivariable model predictive control design strategy which incorporates manipulated variable blocking, and its computation using the singular value decomposition (SVD) approach. The attraction of the SVD approach is that it is a more reliable and transparent method of computing the solution of unconstrained least-squares optimization problems which often become ill-conditioned for typical tuning and design parameters employed in model predictive control. Guidelines for the application of the SVD approach are presented and discussed.

1 INTRODUCTION

Control system design involves two subtasks(Manousiothakis *et al.,* 1986):

1. selection of a control structure i.e. set of measurements and manipulated variables
2. decision on the structure interconnecting the measured and manipulated variables, along with the control law governing the interconnections.

Williams and Adeniyi (2018a) applied the dynamic resilience analysis technique for selection of the most promising control structures for a tubular ammonia reactor-heat exchanger system. This was undertaken as part of the task of advanced control design for the system. Improved control and operation of the ammonia reactor system is an industrially important goal since the Haber process for production of ammonia is the major process in the manufacture of nitrogenous fertilizers - a vital input for modern farming.

After selecting the most promising control structures, the next step in the controller design process is to decide on the controller structure i.e. the interconnections between the sets of inputs (manipulated variables) and outputs (controlled) variables. This is then followed by the actual design of the control laws based on the selected configuration.

For multi-input, multi-out (MIMO) systems, two choices exist for the controller structure: a *centralized* or *decentralized* controller structure. In the *centralized* controller structure, all the measurements are interconnected to all the manipulated variables and this allows the best achievable performance. In the *decentralized* approach, such as the multi-loop structure, one measurement is connected to only one input. This approach (when properly formulated) is more flexible, has lower communication cost, improved safety/fault tolerance, and easier monitoring and on-line tuning (Arkun, 1986; Manousiothakis *et al.,* 1986). Unfortunately, however, the *decentralized* controller structure is not applicable to non-square systems which is one of the requirements or conditions we wish to be able to address in this work. Furthermore, only the *centralized* controller structure allows the attainments of the best achievable performance. Consequently, we chose a *centralized* controller structure in this study.

In this final stage, the actual controller design i.e. derivation of the control law and selection of the tuning parameters, is to be carried out for the most promising control/measurement structure(s) previously identified in Williams and Adeniyi (2018a). The controller design technique should satisfy the following requirements, amongst others: (1) be easily computed so that undue computational burden is not placed on the process control computer, (2) be easily tuned on-line when necessary, (3) have multivariable features that allow a treatment of square as well as non-square systems, and (4) have excellent performance and robustness characteristics.

A technique that meets all the above criteria is Model Predictive Control (MPC) and is adopted for the actual controller design for the tubular ammonia reactor-heat exchanger system previously considered in Williams and Adeniyi (2018a).

Model Predictive Control (MPC) is used to describe the general class of the relatively new generation advanced control techniques which employ directly, a discrete convolution model of either impulse or step response elements for controller design. The underlying concept of MPC is that the future behaviour of a controlled variable is predicted from the present into the future, using a model of the process, and the value of manipulated variables (inputs) are determined such that the predicted values of the controlled variable is a best fit (in a given sense) to a desired value. For more detailed overview of general MPC, see Camacho and Bordons (1995), Lee (2011), Orukpe (2012) and more recently Levine (2019) and the references therein.

MPC has both feedforward and feedback control in its structure. The task of using the model to predict the changes in output and then determining the input to make the predicted output fit the desired value is the feedforward control of MPC. On the other hand, the task of making the observed output the new starting point is the feedback property of MPC. The effect of plant/model mismatch (which always exist in practice) is taken into account in the determination of the input by making the observed output the new starting point for subsequent prediction, and iteratively carrying out the determination of the input (Takamatsu *et al.*, 1988). Thus, MPC replaces the fixed-structure explicit control law (common in other control techniques) with on-line optimization. This makes it possible to deal easily with (1) square and non-square systems, (2) constraints on the manipulated or and controlled variables, and (3) the failure of actuators. While (2) and (3) are important properties/features of MPC, they are not explicitly addressed in our present study.

When input and other constraints are not addressed in an MPC formulation, the solution for the manipulated input becomes a least-squares optimization problem which can become ill-conditioned for typical design parameter values employed. In standard model predictive control (cf. Garcia and Morari, 1982, 1985; Marchetti et al., 1983), input penalty matrices are used for dealing with the ill-conditioning problem and for reducing the aggressiveness of manipulated variable moves. However, this approach has the principal disadvantage that the particular choice of input penalty matrices needed to properly condition the problem is not at all obvious and must therefore be chosen by trial and error. Thus, the motivation for using the singular value decomposition (SVD) is that it is a more reliable way of handling ill-conditioned or rank deficient least-squares optimization problems (cf. Forsythe *et al.*, 1977). Pan *et al*. (2016) have also employed the singular value decomposition to address the problem of ill-conditioned models in model predictive control problem formulation.

In this current paper (Part I), we present the development/formulation of the MPC problem starting from a state-space model, derivation of the control law and its computation using the Singular Value Decomposition (SVD), and then discuss some guidelines for its application. An abridged version of this work was presented in Williams and Adeniyi (2018b) and applied to the case of 2×2 control structures for a tubular ammonia reactor-heat exchanger system. This current work expands on this to include application to 2×3 (non-square) and 3×3 (square) control structures which are presented in the companion paper (Part II). Comparisons of the performance of the SVD-based model predictive controllers with mutli-loop PI controllers previously reported in the literature are also included in Part II.

2 METHODOLOGY

The design of a model predictive controller involves (Garcia and Prett, 1986; Prett and Garcia, 1988): (1) Identification of a linear dynamic (input/output) model relating the manipulated variables to the outputs of interest, (2) Statement of the control objective(s), and (3) Computation of the control law and closed loop implementation.

The development presented in this paper is concerned with only the unconstrained linear model predictive control problem. We assume that the model is open-loop stable. If this is not so, classical techniques such as proportional output feedback control may be used to first stabilize the system before carrying out the model predictive controller design. Also, it is assumed that the control algorithm is implemented in a sample-data system (such as is suitable for implementation on a digital process control computer) so that discrete-time model of the process is considered in which values are known only at discrete intervals of time k :

$$k\tau \le time \le (k+1)\tau$$

where τ is the sampling time of the system.

2.1 Identification of a Linear Input/Output Model of the Process

Based on the results of control structure analysis reported in Williams and Adeniyi (2018a), the linear systems under consideration are all given by state-space equations of the form:

$$\dot{\mathbf{x}} = \mathbf{A}_1\mathbf{x} + \mathbf{B}_1\mathbf{u} + \mathbf{D}_m\mathbf{d}_m$$
$$\mathbf{y} = \mathbf{C}\mathbf{x} \qquad (1)$$

$\mathbf{x}_0 = \mathbf{0}$, where $\mathbf{x} \in \Re^s$, $\mathbf{u} \in \Re^m$, $\mathbf{d}_m \in \Re^r$, and $\mathbf{y} \in \Re^n$, are the vector of the state, manipulated, measurable disturbances and the output variables, respectively. $\mathbf{A}_1, \mathbf{B}_1, \mathbf{D}_m$, and $\mathbf{C}$ are matrices of appropriate dimensions.

2.1.1 Discretization of the continuous model

Since the model predictive control algorithm is normally implemented in a sample-data system, it is necessary to discretize Eq. (1) into the appropriate form. In a sample-data system such as digital computer control, the output of interest is sampled at finite intervals of time τ and the input applied to the system is constant over each interval. This produces a "stair case" input profile:

$$u(t) = u(k); \quad k\tau \le t \le (k+1)\tau$$

where $k = 0, 1, 2, \ldots$, represent discrete-time interval.
Based on the above, and through a process of simple integration, Eq. (1) can be represented at every discrete interval k, as:

$$\mathbf{x}(k+1) = \mathbf{F}\mathbf{x}(k) + \mathbf{G}\mathbf{u}(k) + \mathbf{G}'\mathbf{d}_m(k)$$
$$\mathbf{y}(k+1) = \mathbf{C}\mathbf{x}(k+1); \;\; \mathbf{x}(0) = \mathbf{0} \qquad (2)$$

where:

$$\mathbf{F} = e^{\mathbf{A}_1\tau}, \quad \mathbf{G} = \int_0^\tau e^{\mathbf{A}_1 t}\mathbf{B}_1 dt, \quad \mathbf{G}' = \int_0^\tau e^{\mathbf{A}_1 t}\mathbf{D}_m dt \qquad (3)$$

and τ is the sample time.
Let

$$\mathbf{H}_i = \mathbf{C}\mathbf{F}^{i-1}\mathbf{G}, \quad \mathbf{H}'_i = \mathbf{C}\mathbf{F}^{i-1}\mathbf{G}' \qquad (4)$$

$\mathbf{H}_i$ is the so-called impulse response coefficient that relates the effects of the manipulated variable (inputs) to the output variables; while $\mathbf{H}'_i$ is the impulse response coefficient that relates the effects of the measured disturbances to the outputs.
For N sufficiently large, $\mathbf{x}(k-N+1) \to \mathbf{x}(0) = \mathbf{0}$, it can easily be shown that:

$$\mathbf{y}(k+1) = \sum_{i=1}^{N}\mathbf{H}_i\mathbf{u}(k-i+1) + \sum_{i=1}^{N}\mathbf{H}'_i\mathbf{d}_m(k-i+1) \qquad (5)$$

For open-loop stable (or stabilised) systems, $\mathrm{H}_i \to 0$ as $i \to \infty$ so that a finite N samples is sufficient to describe the system.

An alternative input/output model using step response coefficients can also be used (Prett and Garcia, 1988; Maurath et al., 1988a,b) as is done in Dynamic Matrix Control (DMC), by defining a change in inputs as follows:

$$\Delta\mathbf{u}(k) = \mathbf{u}(k) - \mathbf{u}(k-1) \qquad (6)$$
$$\Delta\mathbf{d}_m(k) = \mathbf{d}_m(k) - \mathbf{d}_m(k-1) \qquad (7)$$

and substituting into Eq. (5). However, in this study, we shall make use of the impulse response model for the control computation.

Let $\mathbf{d}_u(k)$ represent process characteristics such as plant/model mismatch, unmeasurable disturbances (including noise) which are not accounted for in the outputs of the impulse response model; then the process output is given by

$$\mathbf{y}(k+1) = \sum_{i=1}^{N}\mathbf{H}_i\mathbf{u}(k-i+1) + \sum_{i=1}^{N}\mathbf{H}'_i\mathbf{d}_m(k-i+1) + \mathbf{d}_u(k) \qquad (8)$$

2.1.2 The prediction problem

.At time $\bar{k}$, we now use the impulse response model, Eq. (8) to predict future values of the outputs $\mathbf{y}(k)$ over a time horizon, P. Thus, for any future interval of time, the output prediction is given (for a non-zero initial condition, $\mathbf{y}_0$) by

$$\mathbf{y}(\bar{k}+l) = \mathbf{y}_0 + \mathbf{H}_1\mathbf{u}(\bar{k}+l-1) + \mathbf{H}_2\mathbf{u}(\bar{k}+l-2) + \ldots + \mathbf{H}_N\mathbf{u}(\bar{k}+l-N)$$
$$+ \mathbf{H}'_1\mathbf{d}_m(\bar{k}+l-1) + \mathbf{H}'_2\mathbf{d}_m(\bar{k}+l-2) + \ldots + \mathbf{H}'_N\mathbf{d}_m(\bar{k}+l-N)$$
$$+ \mathbf{d}_u(\bar{k}+l), \qquad l = 1, 2, \ldots, P \qquad (9)$$

Let us assume that the measured disturbance variables $(\mathbf{d}_m(\bar{k}+l))$ do not change over the entire future time intervals $(l = 1, 2, \ldots, P)$, but may be measured at the current time, $\bar{k}$, i.e.

$$\mathbf{d}_m(\bar{k}) = \mathbf{d}_m(\bar{k}+1) = \ldots = \mathbf{d}_m(\bar{k}+P) \qquad (10)$$

then, Eq. (9) can be re-written as

$$\mathbf{y}(\bar{k}+l) = \sum_{j=1}^{l}\mathbf{H}_j\mathbf{u}(\bar{k}+l-j) + \mathbf{y}^{\Sigma}(\bar{k}+l) + \mathbf{d}_u(\bar{k}+l), \quad l = 1, 2, \ldots, P \qquad (11)$$

where the term $\mathbf{y}^{\Sigma}(\bar{k}+l)$ is given by

$$\mathbf{y}^{\Sigma}(\bar{k}+l) = \mathbf{y}_0 + \sum_{j=l+1}^{N}\mathbf{H}_j\mathbf{u}(\bar{k}+l-j) + \sum_{j=l+1}^{N}\mathbf{H}'_j\mathbf{d}_m(\bar{k}+l-j) + \sum_{j=1}^{l}\mathbf{H}'_j\mathbf{d}_m(\bar{k}) \qquad (12)$$

and is the contribution to the future values $(l = 1, 2, \ldots, P)$ of the outputs due to past inputs (both manipulated and measured disturbance variables) up to time $\bar{k}-1$, and the most recent measured disturbance, $\mathbf{d}_m(\bar{k})$.

In Eq. (11), future unmodelled effects $\mathbf{d}_u(\bar{k}+l)$ are unknown at the present time, $\bar{k}$, and must therefore be estimated. This is done as follows:

For $l=0$ (present-time prediction, $\bar{k}$), Eq. (11) becomes:

$$\mathbf{y}(\bar{k}) = \mathbf{y}^{å}(\bar{k}) + \mathbf{d}_u(\bar{k}) \tag{13}$$

At present time $\bar{k}$, the process output measurement, $y_m(\bar{k})$ is available. Thus, $d_u(\bar{k})$ can be estimated as

$$\mathbf{d}_u(\bar{k}) = \mathbf{y}_m(\bar{k}) - \mathbf{y}^{å}(\bar{k}) \tag{14}$$

where

$$\mathbf{y}^{å}(\bar{k}) = y_0 + \sum_{j=1}^{N}\mathbf{H}_j\mathbf{u}(\bar{k}-j) + \sum_{j=1}^{N}\mathbf{H}'_j\mathbf{d}_m(\bar{k}-j) \tag{15}$$

is obtained from Eq. (12) by setting $l=0$. Although $\mathbf{d}_u(\bar{k}+l), l=1,2,\ldots,P$ may now be estimated by filtering theory (provided that there is additional knowledge about the noise statistics), the simplest approach is to set (cf. Garcia, 1984; Garcia and Prett, 1986; Prett and Garcia, 1988):

$$\mathbf{d}_u(\bar{k}+l) = \mathbf{d}_u(\bar{k}), \quad l=1,2,\ldots,P \tag{16}$$

which essentially matches the prediction at $\bar{k}$ to the present measurement, $\mathbf{y}_m$.

Substituting Eq. (16) into Eq. (11) we have

$$\mathbf{y}(\bar{k}+l) = \sum_{j=1}^{l}\mathbf{H}_j\mathbf{u}(\bar{k}+l-j) + \mathbf{y}^{å}(\bar{k}+l) + \mathbf{d}_u(\bar{k}), \quad l=1,2,\ldots,P \tag{17}$$

2.2 Statement of the Control Objective

Qualitatively, the control problem to be solved at time $\bar{k}$, is to determine the present [$u(\bar{k})$] and future values of the manipulated variables:[$\mathbf{u}(\bar{k}+l), l=1,2,\ldots,P-1$] such that the predicted future values of the outputs: $\mathbf{y}(\bar{k}+l), l=1,2,\ldots,P$ track the corresponding future set points, $\mathbf{y}_s(\bar{k}+l), l=1,2,\ldots,P$ in an optimal manner.

Mathematically, the present and future values of the manipulated inputs, $\mathbf{u}(\bar{k}+l), l=1,2,\ldots,P-1$ are to be determined by solving the following optimization problem:

$$\min_{\mathbf{u}(\bar{k}+l), l=1,2,\ldots,P-1} \sum_{l=1}^{P}\left[\left\|\mathbf{y}_s(\bar{k}+l)-\mathbf{y}(\bar{k}+l)\right\|^2_{\Gamma_l^T\Gamma_l} + \left\|\mathbf{u}(\bar{k}+l-1)\right\|^2_{\Lambda_l^T\Lambda_l}\right] \tag{18}$$

subject to Eq. (17); in which

$$\|\mathbf{z}\|_R^2 = \mathbf{z}^T\mathbf{R}\mathbf{z}$$

$\mathbf{\Gamma}_l$ and $\mathbf{\Lambda}_l$ are positive semi-definite weighting matrices which are taken to be diagonal in our present study.

If Eq. (17) is written for all future times from $(\bar{k}+1), (\bar{k}+2), \ldots, (\bar{k}+P)$, we obtain the following values of the predicted outputs (after rearrangement into vector-matrix form):

$$\mathbf{Y} = \mathbf{X}\mathbf{U} + \mathbf{Y}^{å} + \mathbf{D}_u \tag{19}$$

where

$$\mathbf{Y} = \left[\mathbf{y}(\bar{k}+1)\ \ \mathbf{y}(\bar{k}+2)\cdots\ \mathbf{y}(\bar{k}+P)\right]^T;\ \mathbf{Y}\in\Re^{np};$$

$$\mathbf{U} = \left[\mathbf{u}(\bar{k})\ \ \mathbf{u}(\bar{k}+1)\cdots\ \mathbf{u}(\bar{k}+P-1)\right]^T, \quad \mathbf{U}\in\Re^{mp}$$

$$\mathbf{Y}^{å} = \left[\mathbf{y}^{å}(\bar{k}+1)\ \ \mathbf{y}^{å}(\bar{k}+2)\cdots\ \mathbf{y}^{å}(\bar{k}+P)\right]^T,$$

$$\mathbf{Y}^{å}\in\Re^{np};\quad \mathbf{D}_u = \left[\mathbf{d}_u(\bar{k})\ \ \mathbf{d}_u(\bar{k})\cdots\ \ \mathbf{d}_u(\bar{k})\right]^T \in\Re^{np}$$

and $\mathbf{X}$ is a lower block-triangular matrix, given by

$$\mathbf{X} = \begin{bmatrix} \mathbf{H}_1 & \mathbf{0} & & \\ \mathbf{H}_2 & \mathbf{H}_1 & \mathbf{0} & \\ \vdots & \vdots & \ddots & \\ \mathbf{H}_P & \mathbf{H}_{P-1} & \cdots & \mathbf{H}_1 \end{bmatrix};\ \mathbf{X}\in\Re^{np\times mp} \tag{20}$$

If we define

$$\mathbf{Y}_s = \left[\mathbf{y}_s(\bar{k}+1)\ \ \mathbf{y}_s(\bar{k}+2),\ldots\ \mathbf{y}_s(\bar{k}+P)\right]^T,\ \mathbf{Y}_s\in\Re^{np}$$

then we can write the following unconstrained quadratic optimization problem

$$\min_{\mathbf{U}}\left[\left\|\mathbf{Y}_s - (\mathbf{X}\mathbf{U}+\mathbf{Y}^{å}+\mathbf{D}_u)\right\|^2_{\Gamma^T\Gamma} + \left\|\mathbf{U}\right\|^2_{\mathbf{\Lambda}^T\mathbf{\Lambda}}\right] \tag{21}$$

If we consider blocking of manipulated variables in the formulation of the model predictive control problem (cf. Reid *et al.*, 1980; Mehra *et al.*, 1981; Ricker, 1985), in which we constrain $\mathbf{U}$ by specifying that the manipulated variables are to be held constant over a block of sampling intervals, allowed to change, and then held constant over another block, and so on, then only the first element of U in each block is retained in the definition of $\mathbf{U}$ which now becomes (cf. Ricker, 1985):

$$\mathbf{U}_B^T = \left[\mathbf{U}_{k_1}^T\ \ \mathbf{U}_{k_2}^T\cdots\ \mathbf{U}_{k_q}^T\right] \tag{22}$$

where $k_1, k_2, \ldots, k_q$ indicate the sampling intervals at which each block starts, and are chosen such that

$$\begin{aligned} &k_1 = 0 \\ &k_j < k_{j+1},\ j = 1, 2, \ldots, q-1, \\ &k_q \le P-1 \end{aligned} \qquad (23)$$

Eq. (22) indicates, for example, that

$$\mathbf{U}_{k_1} = \mathbf{U}_{k_1+1} = \cdots = \mathbf{U}_{k_2-1}$$

with the effect that the size of the X matrix will reduce because the columns representing each block must be added together for consistency with the blocked form of $\mathbf{U}$. For example, if $k_2 = 4$ and $k_3 = 7$, the first four columns of matrix $\mathbf{X}$ [Eq. (20)] would be added together, the next three would be added together, etc.

Based on the foregoing considerations, we can formulate our general model predictive control optimization problem as

$$\min_{\mathbf{u}_{k_1}, \mathbf{u}_{k_2}, \ldots, \mathbf{u}_{k_q}} \sum_{l=1}^{P} \left[\begin{aligned} &\left\| \mathbf{y}_s(\bar{k}+l) - \mathbf{y}(\bar{k}+l) \right\|^2_{\Gamma_l^T \Gamma_l} \\ &+ \left\| \mathbf{u}(\bar{k}+l-1) \right\|^2_{\Lambda_l^T \Lambda_l} \end{aligned} \right] \qquad (24)$$

subject to Eq. (17) and

$$\begin{aligned} &u_{k_1} = u_{k_1+1} = \cdots = u_{k_2-1} \\ &u_{k_2} = u_{k_2+1} = \cdots = u_{k_3-1} \\ &\vdots \\ &u_{k_q} = u_{k_q+1} = \cdots = u_{k_P-1} \end{aligned} \qquad (25)$$

As pointed out by Ricker (1985), there are at least two potential advantages to blocking: (1) the dimensionality of the optimization problem can be greatly reduced by the elimination of variables from $\mathbf{U}$, while still retaining a large prediction horizon, P; (2) since blocking affects the form of $\mathbf{X}$, it represents an additional way to tune the controller. The blocking of the manipulated inputs $\mathbf{U}$ (but not the outputs $\mathbf{Y}$) is said to be analogous to using a state-deadbeat controller rather than an output-deadbeat controller which is likely to cause large fluctuations in the manipulated variables, especially for higher-order systems — such as lumped parameter approximants of DPS. Blocking can resolve such a problem. As noted by Ricker (1985, 1990), blocking is a generalization of the manipulated variable suppression parameter used for examples, by Garcia and Morari (1985a,b) and in DMC (Prett and Garcia, 1988). Cagienard *et al.* (2007), Shekhar and Manzie (2015) and Schwickart *et al.* (2016) present some more recent discussions of the benefits and strategies for move blocking in model predictive control.

Let there be q blocks of the manipulated variables at the samples periods: $k_1, k_2, \ldots, k_q$ according to Eq. (23). Then the blocked manipulated variables can be collected together in the vector $\mathbf{U}_b \in \Re^{mq}$ which is related to $\mathbf{U}$ according to the equation

$$\mathbf{U} = \mathbf{T}_b \mathbf{U}_b \qquad (26)$$

where $\mathbf{T}_b \in \Re^{mp \times mq}$ is a matrix of zeros and ones.

2.3 Computation of the Control Law and Implementation

The optimization problem given above is a standard linear least squares problem for which it is possible to easily obtain an analytical solution from the following development.

In terms of the blocked variables, $\mathbf{U}$ is related to $\mathbf{U}_b$ according to Eq. (26), thus, Eq. (19) can be re-written as

$$\mathbf{Y} = \mathbf{X}\mathbf{T}_b\mathbf{U}_b + \mathbf{Y}^{*} + \mathbf{D}_u \qquad (27)$$

in which

$$\mathbf{U}_b = \begin{bmatrix} \mathbf{u}_{k_1}^T & \mathbf{u}_{k_2}^T & \cdots & \mathbf{u}_{k_q}^T \end{bmatrix} \in \Re^{mq}$$

Then in terms of the blocked manipulated inputs $\mathbf{U}_b$, Eq. (21) is equivalent to the following unconstrained quadratic optimization problem

$$\min_{\mathbf{U}_b} \left[\left\| \mathbf{E} - \mathbf{X}\mathbf{T}_b\mathbf{U}_b \right\|^2_{\Gamma^T\Gamma} + \left\| \mathbf{T}_b\mathbf{U}_b \right\|^2_{\Lambda^T\Lambda} \right] \qquad (28)$$

where

$$\mathbf{E}(\bar{k}+1) = \mathbf{Y}_s - \mathbf{D}_u - \mathbf{Y}^{*} = \left[\mathbf{Y}_s - \mathbf{D}_u \right] - \left[\mathbf{Y}^{*} \right] \qquad (29)$$

Eq.(28) has the well-known least-squares solution given by

$$\mathbf{U}_b = \left[\mathbf{T}_b^T\mathbf{X}^T\Gamma^T\Gamma\mathbf{X}\mathbf{T}_b + \mathbf{T}_b^T\Lambda^T\Lambda\mathbf{T}_b \right]^{-1} \mathbf{T}_b^T\mathbf{X}^T\Gamma^T\Gamma\mathbf{E}(\bar{k}+1) \qquad (30)$$

$$= \left[\mathbf{X}_b^T\mathbf{X}_b + \mathbf{T}_b^T\Lambda^T\Lambda\mathbf{T}_b \right]^{-1} \mathbf{X}_b^T\mathbf{E}(\bar{k}+1) \qquad (31)$$

where $\mathbf{X}_b = \Gamma\mathbf{X}\mathbf{T}_b$.

In the above equations/expressions, n is the number of output variables; m is the number of manipulated inputs, and P is the controller prediction horizon. We note that in this formulation, the number of inputs (m) may not necessarily be equal to the number of output variables (n).

2.3.1 Computation of control law using the singular Value decomposition (SVD)

If the matrix $\mathbf{X}_b$ has full rank i.e. Rank$[\mathbf{X}_b] = mq$ (where $mq \le np$) then the solution to the optimization problem is unique and can be reliably computed using Eq. (31). The assumption that $\mathbf{X}_b$ has full rank has been implicitly made in writing the solution as Eq. (31). However, when matrix $\mathbf{X}_b$ is rank deficient (i.e. Rank $[\mathbf{X}_b] = k < mq)$ or nearly so, the solution $\mathbf{U}_b$ cannot be reliably computed using Eq. (31) because of ill-conditioning i.e. small changes in the elements of matrix $\mathbf{X}_b$ can result in large changes in the elements of the solution, $\mathbf{U}_b$. Furthermore, the solution $\mathbf{U}_b$ is then not unique. However, uniqueness is obtained by picking the shortest such solution (Forsythe *et al.*, 1977). The ill-conditioning problem occurs as the dimensions of the matrix $\mathbf{X}_b$ increases, especially for values of P and q parameters usually used for predictive controller designs.

The input penalty matrices, $\mathbf{\Lambda}_l, l = 1, 2, \ldots, P$ are used in standard model predictive control (cf. Garcia and Morari, 1982, 1985; Marchetti *et al.*, 1983) for dealing with the ill-conditioning problem and for reducing the manipulated variable moves much similar to the way the ridge parameter is used in ridge regression for statistical parameter estimation problems (Ogunnaike, 1983; 1986). However, this approach has the principal disadvantage that the particular choice of Λ_l needed to properly condition the problem is not at all obvious and must therefore be chosen by trial and error. For this reason, we set $\mathbf{\Lambda}_l = 0, l = 1, 2, \ldots, P$.

A more reliable way of handling ill-conditioned or rank deficient least-squares optimization problems is through the application of the singular value decomposition, SVD (cf. Forsythe *et al.*, 1977).

By employing the singular value decomposition (SVD) of a real matrix $\mathbf{X}_b \in \Re^{nP\times mq}$ defined as follows (cf. Forsythe *et al.*, 1977; Garbow *et al.*, 1977; Dongarra *et al.*, 1979; Klema and Laub, 1980)

$$\mathbf{X}_b = \mathbf{Q}_1 \mathbf{\Sigma} \mathbf{Q}_2^T \qquad (32)$$

where $\mathbf{Q}_1 \in \Re^{nP\times nP}$, $\mathbf{Q}_2 \in \Re^{mq\times mq}$ are orthogonal matrices, and $\mathbf{\Sigma} \in \Re^{nP\times mq}$ is a matrix with entries $\sigma_{ij} = 0$ if $i \ne j$ and $\sigma_{ii} = \sigma_i \ge 0$, in which the quantities σ_i are the singular values of $\mathbf{X}_b$, and the columns of $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are the *left and right singular vectors*, the solution of Eq. (28) can be put in the following form after some rearrangement:

$$\mathbf{U}_b = \mathbf{Q}_2 \mathbf{\Sigma}^+ \mathbf{Q}_1^T \Gamma \left[\mathbf{Y}_s - \mathbf{D}_u - \mathbf{Y}^{å} \right] \qquad (33)$$

where $\mathbf{\Sigma}^+ \in \Re^{mq\times nP}$ is a matrix with entries $\sigma_{ij}^+ = 0$ if $i \ne j$ and $\sigma_{ii} = \sigma_i^+ \ge 0$, in which

$$\sigma_i^+ = \begin{cases} 1/\sigma_i & i = 1, 2, \ldots, L \\ 0 & i = L+1, L+2, \ldots, mq \end{cases}$$

With the moving horizon concept, only the first m values of the mq manipulated inputs computed from Eq. (33) are implemented on the actual process. When the next feedback measurement becomes available [i.e. new $\mathbf{D}_u(\bar{k}+1)$] the problem is solved again. In this regard, we should particularly note that only the vector $\mathbf{E}(\bar{k}+1) = [\mathbf{Y}_s - \mathbf{D}_u - \mathbf{Y}^{å}]$ in Eq. (33) changes at every sample time.

2.3.2 Controller Tuning and Stability

For systems where $m < n$, or for constrained systems where $m \ge n$, it may not be possible to achieve the desired control objective.

Garcia and Morari (1982, 1985a,b), and several other authors (Ricker, 1985; Maurath *et al.*, 1988a,b; Prett and Garcia, 1988; Erickson and Otto, 1991) have discussed the tuning and stability analysis of model predictive control algorithms. Because model predictive controllers have an internal model control structure (Garcia and Morari, 1982), stability of the controller is sufficient for closed-loop stability, provided the model is perfect and open-loop stable.

2.3.3 Computation of Multivariable Off-set Compensator

Finally, it should be pointed out that as fewer number of singular values are retained in the control law given by Eq. (33), the closed-loop system response becomes more sluggish and a point is latter reached when the controller is not able to eliminate offsets. Since integral action is achieved automatically (within the IMC framework) by making the steady-state controller gain the inverse of the model gain (Garcia and Morari, 1982, 1985a,b), it implies that offsets will result when

$$\mathbf{G}(1)\mathbf{G}_I(1) \ne \mathbf{I}$$

where $\mathbf{G}(1)$ is the steady-state gain of the model z-transfer function, while $\mathbf{G}_I(1)$ is the steady-state gain of the controller z-transfer function. This problem is corrected by the use of the multivariable offset compensator proposed by Garcia and Morari (1985b):

$$\mathbf{G}_{OFF} = \left[\mathbf{G}(1)\mathbf{G}_I(1)\right]^{-1} \tag{34}$$

2.4 SVD Application Guidelines to MPC Controller Design

Most applications of the SVD require the specification of a tolerance or zero threshold, $\sigma^{å}$ for which Garbow *et al.* (1977) and Forsythe *et al.* (1977) recommend the following:

1. In problems involving experimental or inexact data

$$\sigma^{å} \geq \max_{i,j} |\Delta_{ij}| \tag{35}$$

where Δ_{ij} are errors in the elements of the matrix whose SVD is being computed.

2. For problems whose matrix elements are known exactly, or are contaminated only by round-off error:

$$\sigma^{å} \geq \sqrt{nP \times mq}\, ò \max_j \sigma_j \tag{36}$$

where $ò$ is the relative accuracy of the floating point arithmetic on the machine being used.

Following the specification of $\sigma^{å}$, the *effective rank* of the matrix $\mathbf{X}_b \in \Re^{nP\times mq}$ is the number of singular values which are greater than $\sigma^{å}$. If the effective rank of $\mathbf{X}_b$ is mq, then the matrix is of "full rank".

The SVD can be applied directly to the optimization problem as follows:

$$\rho(\mathbf{U}_b) = \min_{\mathbf{U}_b} \left\|\mathbf{E} - \mathbf{X}\mathbf{T}_b\mathbf{U}_b\right\|^2_{\mathbf{\Gamma}^T\mathbf{\Gamma}} \tag{37}$$

$$= \min_{\mathbf{U}_b} \left\|\mathbf{X}_b\mathbf{U}_b - \mathbf{\Gamma}\mathbf{E}\right\|^2 \tag{38}$$

$$= \min_{\mathbf{U}_b} \left\|\mathbf{Q}_1\mathbf{\Sigma}\mathbf{Q}_2^T\mathbf{U}_b - \mathbf{\Gamma}\mathbf{E}\right\|^2 \tag{39}$$

where $\mathbf{E}(\bar{k}+1)$ has been replaced with $\mathbf{E}$ for notational convenience only; and $\mathbf{X}_b = \mathbf{\Gamma}\mathbf{X}\mathbf{T}_b$ has been replaced by its SVD in Eq. (39).

Since orthogonal matrices preserve norm i.e.

$$\text{P}\mathbf{Q}_1^T\mathbf{x}\text{P}=\text{P}\mathbf{x}\text{P}$$

We can multiply Eq. (39) by $\mathbf{Q}_1^T$ without changing its norm, to obtain

$$\rho(\mathbf{U}_b) = \min_{\mathbf{U}_b} \left\|\mathbf{Q}_1^T\mathbf{Q}_1\mathbf{\Sigma}\mathbf{Q}_2^T\mathbf{U}_b - \mathbf{Q}_1^T\mathbf{\Gamma}\mathbf{E}\right\|^2 \tag{40}$$

$$= \min_{\mathbf{U}_b} \left\|\mathbf{\Sigma}\mathbf{Q}_2^T\mathbf{U}_b - \mathbf{Q}_1^T\mathbf{\Gamma}\mathbf{E}\right\|^2 \tag{41}$$

If we define the following:

$$\mathbf{w} = \mathbf{Q}_2^T\mathbf{U}_b \tag{42}$$

$$\mathbf{g} = \mathbf{Q}_1^T\mathbf{\Gamma}\mathbf{E} \tag{43}$$

Eq. (41) becomes

$$\rho(\mathbf{U}_b) = \min_{\mathbf{U}_b} \left\|\mathbf{\Sigma}\mathbf{w} - \mathbf{g}\right\|^2$$

$$= \min_{\mathbf{U}_b} \left\|\mathbf{\Sigma}\mathbf{w} - \mathbf{g}\right\| \tag{44}$$

since minimizing the square of the length is equivalent to minimizing the length itself. The vector $\mathbf{w}$ is known as the principal components in the literature (cf. Maurath *et al.*, 1988; Callaghan and Lee, 1988).

Thus, the application of the SVD reduces the least-squares problem to one involving an essentially diagonal matrix, $\mathbf{\Sigma}$.

When $\mathbf{X}_b$ is of rank k relative to $\sigma^{å}$, the *minimal norm* vector w, that solves the optimization problem [Eq. (44)] is given by (cf. Forsythe *et al.*, 1977):

$$w_j = \frac{g_j}{\sigma_j},\ \ \sigma_j \neq 0,\ \ j = 1, 2, \text{K}, k$$

$$w_j = 0,\ \ \sigma_j < \sigma^{å},\ \ j = k+1, k+2, \text{K}, mq \tag{45}$$

Then, $\mathbf{U}_b$ is obtained from

$$\mathbf{U}_b = \mathbf{Q}_2\mathbf{w} \tag{46}$$

Eq. (45) shows that $w_j,\ j = 1, 2, \text{K}, k$, are solved exactly. The remaining ones lead to a possibly non-zero residual given by

$$\rho_k = \sum_{j=k+1}^{nP} g_j^2 = \sum_{j=1}^{nP} g_j^2 - \sum_{j=1}^{k} g_j^2 \tag{47}$$

Or, equivalently,

$$\bar{\rho}_k = \frac{\sum_{j=k+1}^{nP} g_j^2}{\sum_{j=1}^{nP} g_j^2} = 1 - \frac{\sum_{j=1}^{k} g_j^2}{\sum_{j=1}^{nP} g_j^2} \tag{48}$$

where ρ_k has been normalized to $\bar{\rho}_k$ by the largest possible residual which would occur if no singular value is included in the solution vector i.e. $\sum_{j=1}^{nP} g_j^2$, which is the largest possible residual if all the solution components $w_j,\ j = 1, 2, \ldots, mq$ are set to zero.

To compute ρ_k (or equivalently, $\bar{\rho}_k$), it is necessary to specify $\mathbf{E}$. Under closed-loop control, $\mathbf{E}$ changes at every sample time and this change cannot be determined apriori. Hence, for the purpose of computing ρ_k (or $\bar{\rho}_k$), we assume a simultaneous unit step change in all the outputs i.e. $\mathbf{E}$ is taken as

$$\mathbf{E} = (1\ 1\ldots\ 1 1\ 1\ldots\ 1\ldots\ 1\ 1\ldots\ 1)^T \in \Re^{nP\times 1} \tag{49}$$

The sensitivity of the solution ($\mathbf{U}_b$) to errors in X_b is well known to be given by

$$\eta_L(X_b) = \frac{\sigma_1}{\sigma_L} \tag{50}$$

where σ_1 is the maximum singular value, and σ_L is the smallest singular value of the matrix $\mathbf{X}_b$ with effective rank, L.

The quantities, η_L and $\bar{\rho}_L, L = 1, 2, \ldots, k$, can be readily computed from the SVD matrices, and on the basis of their values, the designer may decide on the number of singular values to retain in the solution. A table can be constructed to aid the designer by listing the following:

1. The singular values of $\mathbf{X}_b$, $\sigma_i, i = 1, 2, \ldots, k$, where k is the effective rank of $\mathbf{X}_b$.
2. The condition number, η_L, assuming L number of singular values (arranged in descending order of magnitude) are retained in the solution i.e. $\eta_L = \sigma_1 / \sigma_L$.
3. The residual, ρ_L or $\bar{\rho}_L$, assuming L number of singular values (arranged in descending order of magnitude) are retained in the solution and the rest discarded.

3 DISCUSSIONS

The above completes the controller design strategy. To round up, let us state as follows: Joseph and Brosilow (1975) have earlier used the condition number and the residual ($\bar{\rho}$) as criteria for the selection of secondary measurements for inferential control of processes, for which a least-squares problem was formulated. They recommend a residual, $\bar{\rho} \le 0.05$, and a condition number, $\eta < 100$. However, they did not use the SVD technique as we have proposed here. Let us also state that Maurath *et al.* (1988b) have presented a principal component analysis (PCA) method for the design of a model predictive controller (such as DMC) using the SVD technique. The approach presented in this work, while similar to the approach of Maurath *al.* (1988b) in the use of the SVD technique, is entirely different and more straightforward.

4 CONCLUSION

This paper presented a multivaiable model predictive control design strategy which incorporated a general manipulated variable blocking and its computation using the singular value decomposition (SVD) approach. Guidelines for the application of the SVD approach were presented and discussed. The approach has been successfully applied to evaluate various 2×2, 2×3 and 3×3 control structures for a tubular ammonia reactor-heat exchanger system under nominal, additive plant/model mismatch and measurement noise. The results are presented in the companion paper (Part II) of this work.

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