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AN ALGORITHM FOR SET-POINT OPTIMIZATION*

Introduction

A new algorithm for set-point optimization is presented. The available models of industrial processes, as a rule, include unknown deterministic or random parameters. The value of these parameters is to be re-estimated, using new information as it becomes available. The suggested algorithm was developed specially for the case of an invalid separation theorem.

The algorithm is based on replacing the customary optimization problem by a free boundary problem. The replacement is valid under not too restrictive assumptions. The resulting partial differential equation with free boundaries is solved, using a numerical method. This method reduces the problem to solving a system of nonlinear polynomial equations at fixed time moments.

The free boundary problem can be solved in the background or during the elaboration of the on-line system. As a result, we get a suboptimal strategy determined by sets in the state space, with known fixed value of control in each set. To compute a set-point value in real time, we have to estimate the state variables and classify the state variable estimates between given sets.

The algorithm cited will be displayed, using the model of the sulphoetherification section of the synthetic detergent tipol production process. The main reaction synthesizing tipol is the addition reaction between sulphuric acid and a certain fraction of distilled oil (crude or shale oil). The main reaction is accompanied by a number of concurrent reactions, such as polymerization, isomerization, oxydation and others. Depending on the conditions of reactions and on the quality of the oil fraction, the effect of concurrent reactions on the quality and quantity of the final product can be significant.

The quality of the oil fraction changes from batch to batch and is neither exactly known nor predictable using prior measurements only. Here arises the necessity for re-estimating the model parameters and for recomputing control values, using new available information. It should be noted that the quality of estimation in our case depends on the control values used: the so-called dual control problem arises since the separation theorem is not valid.

General layout of the control system and the structure of control strategy are illustrated by Figs 1 and 2, respectively.

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1. A model of the sulphoetherification section

We are going to describe the dependence of the output flow of the section on control variables, provided the quality of input flow does not change.

The sulphoetherification process proceeds in a cooled heat exchanger. Reagents are mixed in a feed pump directly before entering the heat exchanger. In the following two reactors the neutralization with alkaline

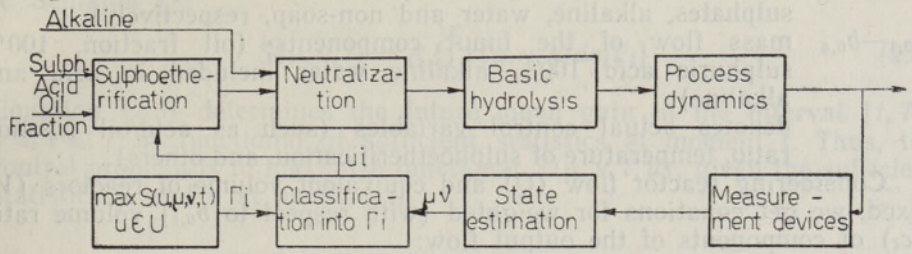

Fig. 1. General layout of the control system: u_i — control variable, μ, ν — sufficient statistics, Γ_i — subset in space of sufficient statistics, where $u_{opt} = u_i$.

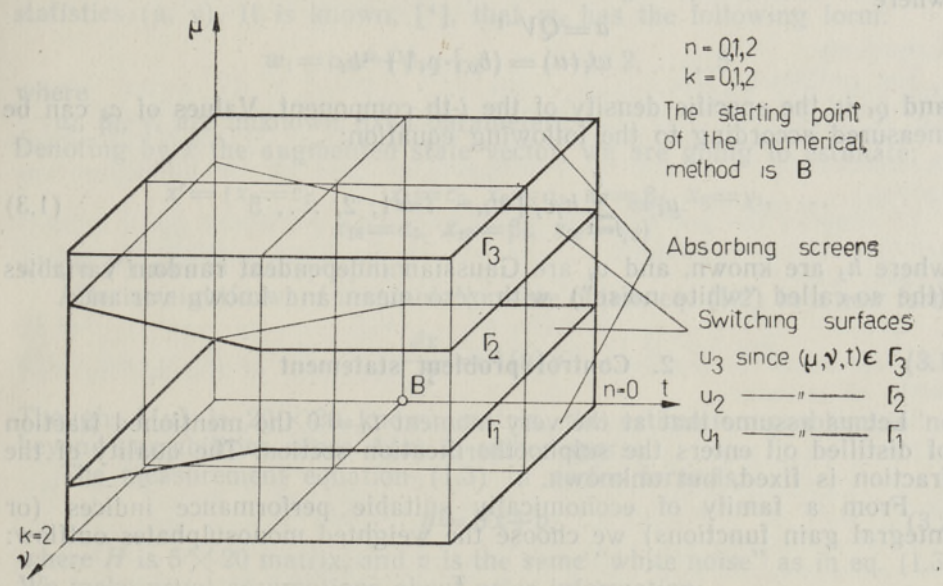

Fig. 2. The structure of the control strategy.

and basic hydrolysis goes on. The reaction time of sulphoetherification and neutralization reactions is short as compared with the delay due to the volume of reactors. With a negligible error, we can describe chemical reaction as inertialess, followed by ideal mixing in equivalent volume of a reactor [1].

In the following we take the flows of the process to consist of a fixed number of components. The qualitative characteristics of these components remain unchanged [2]. Making use of the known structure of mass distribution and considering the mass flow of monosulphates proportional to the mass flow of the oil fraction, we get equations for output components of the inertialess part of the process:

$$\begin{aligned} b_1 &= g_1(u)\, b_{0,1}, \\ b_2 &= g_2(u)\, b_{0,1} + a_2 b_{0,2}, \\ b_3 &= g_3(u)\, b_{0,1} + a_3 b_{0,2} + b_{0,3}, \\ b_4 &= g_4(u)\, b_{0,1} + a_4 b_{0,2} + b_{0,4}, \\ b_5 &= g_5(u)\, b_{0,1} \end{aligned} \tag{1.1}$$

where

$g(u)$ denotes vector of control dependent coefficients;

b_1—b_5 mass flow of the output components (monosulphates, natrium sulphates, alkaline, water and non-soap, respectively);

$b_{0,1}$—$b_{0,4}$ mass flow of the input components (oil fraction, 100% sulphuric acid, 100% alkaline, water included in acid and alkaline);

u denotes actual control variables (such as acid/oil fraction ratio, temperature of sulphoetherification, and others).

Considering reactor flow (Q) and equivalent volume of reactors (V) fixed, we get equations for weighted (with respect to $b_{0,1}$) volume ratio (c_i) of components of the output flow:

$$\frac{dc_i}{dt} + ac_i = w_i(u), \quad i = 1, 2, \ldots, 5 \tag{1.2}$$

where

$$\begin{aligned} a &= QV^{-1} \\ w_i(u) &= (b_{0,1} \cdot \varrho_i V)^{-1} b_i \end{aligned}$$

and ϱ_i is the specific density of the i-th component. Values of c_i can be measured according to the following equation:

$$y_i = \sum_{j=1}^{5} h_j c_j + v_i, \quad i = 1, 2, \ldots, 5 \tag{1.3}$$

where h_j are known, and v_i are Gaussian independent random variables (the so-called "white noise") with zero mean and known variance.

2. Control problem statement

Let us assume that at the very moment $t_0 = 0$ the mentioned fraction of distilled oil enters the sulphoetherification section. The quality of the fraction is fixed, but unknown.

From a family of economically suitable performance indices (or integral gain functions) we choose the weighted monosulphates outflow:

$$L(c_1(u), T) = \int_0^T c_1(u, s)\, ds \tag{2.1}$$

where $u = b_{0,1}^{-1} \cdot b_{0,2}$ is scalar control variable.

Our aim is to maximize (2.1) subject to eq. (1.2) and

$$u_{\min} \leqslant u \leqslant u_{\max}.$$

Unfortunately, due to unknown coefficients w_i in eq. (1.2) and measurement noise v_i in (1.3), immediate maximizing of (2.1) is impossible. Now, let us assume that the unknown parameters have known prior Gaussian probability density. In the following section it is shown that in our case posterior probability density is Gaussian as well. Keeping that in mind, we define momentary posterior gain:

$$r(\mu, \nu, t) = \mathcal{E}\{c_1(w, a, t)/F_t\} \tag{2.2}$$

where

$\mathcal{E}\{\cdot/F_t\}$ denotes conditional mathematical expectation with respect to

$$F_t = \sigma\{y(s), u(s): 0 \leqslant s \leqslant t\},$$

σ-field containing known history of the process. Here μ and ν are mean and variance of the posterior probability density of c_1, in fact sufficient statistics.

Making use of (2.2), we define preposterior gain of H. Raiffa and R. Schlaifer [3]

$$S(\mu, \nu, t) = \mathcal{E}\{\int_t^T r(\mu, \nu, s)\, ds/F_t\}. \tag{2.3}$$

Equation (2.3) determines the future mean gain in the interval $[t, T]$, $0 \leqslant t \leqslant T$ as functional of sufficient statistics at moment t. Thus, the control problem is to maximize functional $S(\mu, \nu, t, u)$, given the sufficient statistics μ and ν at moment t.

3. Equations for sufficient statistics

In this section we write out equations for estimating c_i and w_i $(i = 1, 2, 3, 4, 5)$, and from these equations we get equations for sufficient statistics (μ, ν). It is known, [4], that w_i has the following form:

$$w_i = \alpha_i u^2 + \beta_i u + \gamma_i, \quad i = 1, 2, \ldots, 5$$

where

α_i, β_i, γ_i are unknown fixed parameters.

Denoting by x the augmented state vector, we are going to estimate:

$$x' = (x_1 = c_1, \ldots, x_5 = c_5, x_6 = \alpha_1, x_7 = \beta_1, x_8 = \gamma_1, \ldots, x_{18} = \alpha_5, x_{19} = \beta_5, x_{20} = \gamma_5)$$

where $(')$ means transposition.

After straightforward manipulations we obtain eq. (1.2) in a new form:

$$\frac{dx}{dt} = A(u)x. \tag{3.1}$$

Though $A(u)$ is 20×20 known matrix, the estimation problem is not beyond our abilities, since $A(u)$ is rather sparse.

The measurement equation (1.3) in vector form is:

$$y = Hx + v, \tag{3.2}$$

where H is 5×20 matrix, and v is the same "white noise" as in eq. (1.3). We make usual assumptions about prior information:

i) $x(0) = x_0$ is Gaussian random variable with known probability density $x_0 \sim N(\varkappa_0, K_0)$;

ii) v is "white noise" with nonsingular covariation matrix CC'.

For system (3.1, 3.2), it can be shown under these assumptions that posterior probability density of x is also Gaussian, with mean and covariance satisfying equations (for example [5]):

$$\begin{aligned} \frac{d\varkappa}{dt} &= A(u)\varkappa + KH'(CC')^{-1}(y - H\varkappa), \\ \frac{dK}{dt} &= A(u)K + KA'(u) - KH'(CC')^{-1}HK. \end{aligned} \tag{3.3}$$

In our case eq. (3.3) coincides with Kalman filter equations. Eq. (3.3) gives us parameters of the multidimensional Gaussian density, although in (2.3) we need only marginal density of x_1. The latter is also Gaussian, with mean μ and variance ν. Because of Gaussianity the pair (μ, ν) is sufficient statistic. The equations for μ and ν follow from eq. (3.3).

Note that covariance matrix K depends on used values of control variable. Therefore we cannot separate estimation and control, and dual control problem arises.

4. A free boundary problem

Applying formally dynamic programming, we see that preposterior gain $S(\mu, \nu, t)$ satisfies Bellman's equation

$$-S_t = \max_{u \in U} \{r(\mu, \nu, t, u) + S_\nu d(\nu, t, u) + S_\mu f(\mu, \nu, t, u) + {}^1/_2 S_{\mu\mu} e(\nu, t, u)\} \quad (4.1)$$

where S_t, S_ν, S_μ, $S_{\mu\mu}$ denote, as usual, partial derivatives, and U denotes the set of allowable control values. The coefficients $d(\nu, t, u)$ and $e(\nu, t, u)$ are upper left elements of the matrices

$$D(K, t, u) = AK + KA' - KH'(CC')^{-1}HK$$

and

$$E(K, t, u) = KH'(CC')^{-1}HK,$$

respectively.

The coefficient $f(\mu, \nu, t, u)$ is the first element of the vector $A(u)\varkappa$.

Solving eq. (4.1), even approximately, is extremely laborious. This is caused by nonlinear functions $d(\nu, t, u)$ and $e(\nu, t, u)$. Such difficulties are common in dual control problems (the case of invalid separation theorem).

To simplify the problem, we first restrict the allowable set of control variable values. Henceforth U consists of the final number of control variable values

$$U = \{u_1, u_2, \ldots, u_r\}. \quad (4.2)$$

This restriction is reasonable because of the noise in the system and inertia of actuators.

Secondly, we are not going to solve eq. (4.1) in a whole space of sufficient coordinates (μ, ν, t), since μ is a combination of volume rations (c_i) and coefficients (w_i). Both can assume only bounded values. We introduce the allowable set of sufficient coordinates

$$\Gamma(\mu, \nu, t) = \{(\mu, \nu, t) : m \leqslant \mu \leqslant M, 0 \leqslant t \leqslant T\}. \quad (4.3)$$

Bounds m and M correspond to values of μ that can cause breakdown — i. e. computer transfers control to man-operator who takes care of further decisions. To enable prior or background solution of the control problem, we consider bounds m and M as absorbing screens — once on the screen, μ remains there till T.

With eq. (4.2) in mind, we can replace eq. (4.1) with the system of equations

$$-S_t = r(\mu, \nu, t, u_i) + S_\nu d(\nu, t, u_i) + S_\mu f(\mu, \nu, t, u_i) + {}^1/_2 S_{\mu\mu} e(\nu, t, u_i), \quad i = 1, 2, \ldots, r. \quad (4.4)$$

The maximum property of the overall solution $S(\mu, \nu, t, u)$ of the system is ensured by proper partitioning of the allowable set of sufficient

coordinates Γ, (4.3) into subsets Γ_i, $\Gamma = \bigcup_{i=1}^{r} \Gamma_i$. Note that in Γ_i the value of control variable is fixed and equal to u_i.

We denote boundaries between Γ_i and Γ_j by B_{ij}, and they are actually switching surfaces for control variable. Since switching surfaces are not fixed beforehand, they are called free boundaries. It is clear that in order to maximize (4.4) we have to determine optimal boundaries (switching surfaces).

To provide maximizing property for the free boundaries, we evaluate special discontinuity conditions for $S(\mu, \nu, t)$ on them. For evaluating these conditions, we need the following assumptions:

i) one-side derivatives of $S(\mu, \nu, t, u)$ up to the second degree (incl.) with respect to μ and to the first degree with respect to ν and t exist on switching surfaces;

ii) tangential plane exists for each point $(\mu_0, \nu_0, t_0) \in B_{ij}$; we also assume that B_{ij} has continuous second derivative with respect to μ;

iii) increments of μ behave well: their means and variances do not grow too fast in time.

Under assumptions (i—iii), we are able to prove [6] that on any fixed switching surface

$$S^i_\mu = S^j_\mu, \qquad (\mu, \nu, t) \in B_{ij}, \tag{4.5}$$

and on the optimal switching surface

$$S^i_{\mu\mu} = S^j_{\mu\mu}, \qquad (\mu, \nu, t) \in B_{ij}. \tag{4.6}$$

Upper indices denote the one-side derivative from corresponding subset. From definition of the preposterior gain (1.3), we conclude that

$$S^i = S^j \tag{4.7}$$

on any fixed switching surface. On the absorbing screen we can use typical condition

$$S(\bar{\mu}, \nu, t) = \int_t^T r(\bar{\mu}, \nu, s)\, ds \tag{4.8}$$

where $\bar{\mu} = m$ or $\bar{\mu} = M$. Applying again eq. (1.3), we get

$$S(\mu, \nu, T) = 0. \tag{4.9}$$

Summing up all conditions, we see that instead of the problem of solving Bellman's equation we have the following free boundary problem: solve the system of equations (4.4) with discontinuous coefficients in Γ. On absorbing screens we have boundary conditions (4.8), and on the plane $t = T$ initial conditions (4.9). The surfaces where coefficients have discontinuities, are neither fixed nor known. For simultaneous evaluation of switching surfaces and solution of eq. (4.4) we have conditions (4.5—4.9).

It is important to notice that the solution of the above free boundary problem is independent of measurements. We can solve it beforehand on large computers, provided we know the parameters μ_0 and ν_0.

5. An algorithm solving the free boundary problem

Our free boundary problem differs from the Stefan problem, well known in mathematical physics [7] and sequential analysis [8,9]. Main differences are:

i) discontinuity conditions (4.5, 4.6) do not explicitly include derivative of the free boundary;
ii) value of the preposterior gain on the free boundary is unknown (condition (4.7)).

Because of these differences, we cannot use the numerical methods developed for the Stefan problem. The method suggested in this report is based on [10,11,12]. According to the method, we replace derivatives with respect to t and ν by difference quotients:

$$\frac{\partial S^i}{\partial t}\Big/_{t=n\Delta} = \frac{1}{\Delta}[S^i_{nk} - \tilde{S}^i_{(n-1)k}], \quad n=0, \ldots, N \tag{5.1}$$

$$\frac{\partial S_i}{\partial \nu}\Big/_{\nu=kh} = \frac{1}{h}[S^i_{nk} - \hat{S}^i_{n(k-1)}], \quad k=0, \ldots, K$$

where Δ is the time increment and h is the variance increment. From now on the upper index i denotes that $(\mu, \nu, t) \in \Gamma_i$ and lower indices n and k denote a particular mesh point. Functions $\tilde{S}^i_{(n-1)k}$ and $\hat{S}^i_{n(k-1)}$ are solutions of eq. (5.2) in previous mesh points, extended suitably for use in (5.1, 5.2).

In each mesh point we have to solve the ordinary differential equation

$$\tfrac{1}{2}\frac{\partial^2 S^i_{nk}}{\partial \mu^2} e(k, n, u_i) + \frac{\partial S^i_{nk}}{\partial \mu} f(\mu, k, n, u_i) + r(\mu, k, n, u_i) +$$

$$+ \frac{1}{h}(S^i_{nk} - \hat{S}^i_{n(k-1)})\, d(k, n, u_i) + \frac{1}{\Delta}(S^i_{nk} - \tilde{S}^i_{(n-1)k}) = 0, \quad i=1, 2, \ldots, r. \tag{5.2}$$

Note that subsets Γ_i on the three-dimensional space decay into intervals Γ_{ink}. Our task is now to evaluate switching points and at the same time solve eq. (5.2).

In general it is not possible to get a solution of eq. (5.2) in elementary functions. So we look for a solution in the form of truncated power series

$$S^i_{nk} = \sum_{s=0}^{p} \alpha^i_{snk} \mu^s$$

where α^i_{0nk} and α^i_{1nk} are constants of integration, and p determines the quality of approximation.

Solution of eq. (5.2) in the intervals Γ_{ink}, $i = 1, 2, \ldots, r$ are to be fitted together so as to satisfy conditions (4.5—4.8). The desired result may be acquired by suitable selection of constants of integration and end points of the intervals [12]. For their evaluation we form a system of polynomial equations based on conditions (4.5—4.8). The system of equations consists of $(r-1) \times 3 + 2$ equations, and we have to solve it in each mesh point.

Consider, for example, the case $r = 3$; this means that we have three control variable values and respectively three subsets Γ_1, Γ_2, Γ_3. Now we get in each mesh point eight polynomial equations, two of which arise from conditions (4.8) on the absorbing screens. On both of the switching points we get three equations, arising from conditions (4.5—4.7). The unknowns are two switching points and two constants of integration

in each interval Γ_{ink}. The process starts in mesh point $n=1$, $k=0$ (see Fig. 2). Note that for $n=0$, i. e. $t=T$ we have $S=0$ and assume that

$$\frac{\partial S}{\partial v}\Big/_{v=0}=0.$$

6. Conclusion

The procedure of replacing the customary optimization problem by a free boundary problem is but one possible way to overcome difficulties that arise with real-time control in case of invalid separation theorem.

We stress that the most laborious part of the suggested algorithm — determination of the suboptimal control strategy by solving the free boundary problem — can be accomplished in the background or by using general-purpose computers. The time demand for the estimation and classification of the estimates can be satisfied in real time. This is the practical advantage of the algorithm.

Some more remarks about the application will be useful. Firstly, at present we are not able to solve the free boundary problem for every possible process model and performance index. The problems with one control variable and performance index containing either one of the state variables (the case of tipol production control) or their linear combination, are handled readily.

Another restriction suggested by the algorithm is the final number of control variable values. Appropriate number of control values should be determined by tradeoff between the required computing time and the control accuracy needed.

Thirdly, our algorithm is given for the case where measurements are continuous in time. This, however, is not the case in industry. Measurements in discrete time result in a change of the filter equations (3.3). Since the suboptimal strategy is discrete in time anyway, we have only to take care of proper timing.

We confess to not having discussed the problem of approximation of the switching surfaces and classification of the estimates into subsets Γ_i. As it is, the selection of these algorithms depends significantly on the particular control computer.

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REŽIIMI OPTIMEERIMISEST SIDUSSÜSTEEMIS

Traditsiooniline stohhastilise juhtimise probleem, mida käsitletakse seoses sünteetiliste pesemisvahendite tootmisprotsessi ühe osa mudeliga, taandatakse vaba rajaga diferentsiaalvõrrandi lahendamiseks. Rajatingimused on tuletatavad preposterioorse riski minimaalsuse nõudest lähtudes.

Vaba raja probleemi võib lahendada võimsal arvutil võtte abil, mis põhineb sirgete meetodil. Juhtimisarvutil, s. o. reaalajas, hinnatakse protsessi olekut ja liigitatakse saadud hinnangud varem leitud klassidesse, mis määravadki juhttoime väärtuse.

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АЛГОРИТМ ДЛЯ ОПТИМИЗАЦИИ ТЕХНОЛОГИЧЕСКОГО РЕЖИМА В РЕАЛЬНОМ ВРЕМЕНИ

Предлагается новый алгоритм стохастического управления неприводимыми системами, в основе которого лежит сведение задачи оптимального управления к решению дифференциального уравнения со свободными границами. Условия для определения свободных границ выводятся из требования минимума препостериорного риска.

Для решения приведенной задачи управления используется численный метод, основанный на идее метода прямых. Полученные свободные границы — поверхности переключения значения управляющего воздействия — определяют закон управления как функцию от наблюдений. При работе в реальном времени необходимо оценить текущее состояние и по ранее вычисленному закону управления установить значение переменной управления.

Вывод алгоритма управления приводится на примере модели одного участка производства синтетического моющего вещества — типола.