Optimal off-line measurement schedule to support process and quality management
Proceedings of European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

Optimal off-line measurement schedule to support process and quality management

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Abstract

Laboratory and other off-line measurements are an integral part of process and quality management. Quite commonly, quality variables measured are statistically dependent and thus measurement of one variable is an indirect measurement of the others. In this presentation we formulate the cost-optimal measurement scheduling problem of laboratory measurements under the constraint that uncertainty in quality variable estimates are at all times less than specified. We solve this problem for Gaussian joint probability density of quality variables and uncertainty evolving according to Ornstein-Uhlenbeck process. In this case the optimal schdule is independent on the measurement values obtained and thus it is a policy. We also discuss other practically relevant formulations of optimal measurement scheduling, in particular ones that link scheduling directly to operative decisions about the process and product quality.

Keywords: quality management, scheduling, optimization, stochastic differential equations, simulated annealing

1. Introduction

Quality management of industrial large-scale processes is typically based on three-level measurement hierarchy: on-line sensors sampled at high frequency, at-line analyzers, and accurate and standardized laboratory measurements. Closed-loop control is based on on-line sensors, but as these are rather indirect measurements and may, e.g., drift, they must be continuously validated. At-line analyzers mimic laboratory analyses but are often not fully compliant with measurement standards. At line analyzers support dynamic validation of on-line measurements and manual quality control. Laboratory analyses are accurate but too infrequent to capture relevant process or quality dynamics and rather expensive to carry out. Laboratory analyses support dynamic validation of at-line analyzers.

At least tens of quality parameters are measured in industrial processes, such as those of papermaking industry. However, the actual quality space is expected to be of much lower dimensionality. Thus quality parameters are typically statistically dependent and measuring a subset of them provides information about the others. Utilizing covariance of quality parameters improves cost-information performance of a measurement system.

The three level measurement hierarchy has evolved rather gradually in process industries, e.g in papermaking industry, and its composition has rarely been optimized to provide the required information at minimum cost. In this presentation we shall discuss how to set up such an optimization problem and discuss its solution when information dynamics is linear-Gaussian. In particular, we shall consider scheduling at-line analyzers and/or laboratory measurements to maintain uncertainty about quality constrained below a prescribed level.

Our approach is based on work by Mehra (1976), and Bicchi and Canepa (1993) who discuss the optimization of measurement scheduling to minimize a weighted covariance matrix on measurement information, see also Gupta et al (2006). In a seminal paper Maier et al (1967) integrated measurement selection and scheduling as degrees of freedom into model-based control optimization. In this presentation we shall formulate the general optimal measurement scheduling problem and solve it with simulated annealing (see e.g. Otten and can Ginneken). Practical applications to papermaking industry are presented in Konkarikoski and Ritala (2006), Gren et al (2007a, 2007b, 2007c).

This paper is organized as follows. In Section 2 we present first the information dynamics in general form and then the linear-Gaussian form (Ornstein-Uhlenbeck process, OUP). For the OUP the time dependence of information uncertainty matrix can be solved analytically and it is independent on the actual measurement values obtained. In Section 3 we motivate and formulate the measurement scheduling problem as a cost minimization task constrained by maximum allowable uncertainty about quality. We note that in the case of linear-Gaussian information dynamics this is a policy optimization: measurement schedule is to be optimized once and for all, independent on measurement values obtained. In Section 4 we discuss solving the optimization problem by applying simulated annealing, and provide examples. In section 5 we discuss alternative optimization formulations, in particular ones that define directly the management/control performance as the objective. We also discuss our experience in applying the measurement scheduling method in practise: e.g. how to infer the “maximum allowable uncertainty” in quality information.

2. Information dynamics

2.1. General case

We shall describe the information about quality parameter $y \in R^m$ at time *t*, given a measurement history $mh(t) = \left\{ \left\{ x^{(j)}(t^{(i_j)}) \right\}_{i_j=1}^{I_j(t)} \right\}_{j=1}^{m}, \quad t^{(i_j)} \le t$, with a conditional probability density (notation: capital letters refer to random variables and small letters to their values):

$$f_{Y(t)|mh(t)}\left(y(t) \,|\, \left\{ \left\{ x^{(j)}(t^{(i_j)}) \right\}_{i_j=1}^{I_j(t)} \right\}_{j=1}^{m} \right) \quad (1).$$

Measurement of each quality variable is described as conditional probability densities, too:

$$f_{X^{(j)}|y^{(j)}}\left(x^{(j)} \,|\, y^{(j)} \right) \quad (2).$$

In what follows, we shall assume that measurement uncertainties are not statistically dependent, i.e the joint probability density of measurements $X^{(j)}(t)$, given $y(t)$, is the product of individual densities of form (2).

Information about quality, Eq. (1), evolves through two mechanisms: between measurements the information becomes continuously more uncertain, whereas when measurements are made, the uncertainty about quality is reduced discontinuously.

We choose to describe information degradation with a stochastic differential equation (SDE):

$$dY = F(Y,t)dt + G(Y,t)dW \quad (3),$$

where *W* is an *m*-dimensional Wiener process. Given an initial probability density of *Y* at time t_0, any later probability density is obtained by solving the corresponding Fokker-Planck equation:

$$\frac{\partial f_Y}{\partial t} = O_{FP}\left[f_Y \right] \quad (4),$$

where $O_{FP}[*]$ is the linear Fokker-Planck operator, see e.g. Risken (1996).

When new measurement information becomes available, the information is updated according to Bayes theory as

$$f_{Y(t)|mh(t+)}\left(y(t) \mid \left\{ \left\{ x^{(j)}(t^{(i_j)}) \right\}_{i_j=1}^{I_j(t+)} \right\}_{j=1}^{m} \right) = N \cdot \left(\prod_{j \in meas(t)} f_{X^{(j)}|y^{(j)}}(x^{(j)}(t) \mid y^{(j)}) \right) \cdot f_{Y(t)|mh(t-)}\left(y(t) \mid \left\{ \left\{ x^{(j)}(t^{(i_j)}) \right\}_{i_j=1}^{I_j(t-)} \right\}_{j=1}^{m} \right) \quad (5),$$

where *mh(-)* and *mh(+)* denote measurement history immediately before, respectively after the measurement at time *t* becomes available, and *meas(t)* is set of measurements made at time *t* providing values $x^{(j)}(t)$.

The general information dynamics, Eqs. (3-5), is formally a Kalman state estimation method with SDE of Eq. (3) as the system model. However, as the goal of the measurement system is to maintain the quality uncertainty below prescribed threshold, the SDE is chosen according to worst-case principle, e.g. random walk diffusion or Ornstein-Uhlenbeck process, rather than by seeking an accurate process model.

2.2. Linear-Gaussian case

Let us assume that measurements are unbiased and their uncertainty is described as a Gaussian:

$$f_{X^{(j)}|y^{(j)}}\left(x^{(j)} \mid y^{(j)} \right) = (2\pi \sigma_{meas}^{(j)\,2})^{-1/2} \exp\left(-\frac{(x^{(j)} - y^{(j)})^2}{2\sigma_{meas}^{(j)\,2}} \right) \quad (6),$$

where $\sigma_{meas}^{(j)}$ is the uncertainty in measuring quality parameter *j*. Let us assume that information dynamics is described with Ornstein-Uhlenbeck process:

$$dY = -B(Y - y_m)dt + dW$$
$$E_W\{W(t)\} = 0 \quad E_W\{W(t)W(t')\} = D|t - t'| \quad (7).$$

Matrix *D* – the diffusion matrix – describes how rapidly the uncertainty grows. To interpret the matrix *B*, let us note that the solution of the corresponding Fokker-Planck equation, with initial Gaussian probability density $N(y|y_0,\Sigma_0)$, is a Gaussian with mean and covariance matrix given as (see, e.g. Risken (1996)):

$$E_{W,Y(0)}\{Y(t)\} = y_m + \exp[-Bt](y_0 - y_m)$$
$$E_{W,Y(0)}\{\delta Y(t)\delta Y(t)^T\} = \Sigma_0 \exp[-2Bt] + \frac{1}{2}DB^{-1}(1 - \exp[-2Bt]) \quad (8).$$

As time tends to infinity, all initial information is lost and we are left with *a priori* information about mean and covariance of quality parameters. According to Eq. (8) $f_{Y(\infty)}(y) = N(y \mid y_m, DB^{-1}/2)$ and hence the relationship between matrix *B*, diffusion matrix *D* and the a priori covariance of quality $\Sigma^{(ap)}$ is

$$B = \Sigma^{(ap)^{-1}} D / 2 \qquad (9).$$

Let us now assume that after measurements made at time *t*, the information about quality is $N(y \mid \hat{y}(t), \Sigma(t))$. Let us assume that a subset $\{x^{(j)}\}_{j=j_2}^{m}$ of measurements becomes available at time *t+Δt*. Then according to Eqs. (5-9) the quality information is Gaussian with mean and covariance given as:

$$\hat{y}(t+\Delta t) =$$

$$\Sigma(t+\Delta t)\left(\left(\Sigma(t) + (\Sigma^{(ap)} - \Sigma(t))\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D \Delta t\right)\right)\right)^{-1} \hat{y}^{(-)}(t+\Delta t) + \begin{bmatrix} 0 & 0 \\ 0 & diag(\sigma_{meas}^{(j)\;-2}) \end{bmatrix} \begin{bmatrix} 0 \\ x(t+\Delta t) \end{bmatrix}\right)$$

$$\hat{y}^{(-)}(t+\Delta t) = y_m + \exp\left(-\Sigma^{(ap)^{-1}} D \Delta t / 2\right)\left(y(t) - y_m\right)$$

$$\Sigma(t+\Delta t) = \left[\left(\Sigma(t) + (\Sigma^{(ap)} - \Sigma(t))\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D \Delta t\right)\right)\right)^{-1} + \begin{bmatrix} 0 & 0 \\ 0 & diag(\sigma_{meas}^{(j)\;-2}) \end{bmatrix}\right]^{-1}$$

(10).

For the optimization problem to be formulated in Section 3, it is important to notice that updating uncertainty covariance is independent on measurement values $\{x^{(j)}(t)\}_{j=j_2}^{m}$ obtained.

3. Formulation of optimal measurement scheduling problem

Uncertainty affects decision making in two ways: firstly the more uncertain the information the lower the quality of decisions in terms of the deterministic objective, and secondly the higher the uncertainty the more important is decision maker's attitude towards risk, i.e. whether she/he is risk-aversive, neutral or opportunistic. The latter effect is formalized by replacing the deterministic objective e.g. with a utility function, adding a risk premium to the objective or constraining the probability of particularly poor values of objective (Rios and Insua 2000, Jokinen et al 2006).

Quality information is utilized in a multitude of decisions. In general, measuring the outcome of decisions and the corresponding actions in terms of money is difficult and thus formulating an objective that combines cost and benefit of measurement information is tedious. Therefore, in this paper we concentrate on a case of guaranteeing a chosen quality of decisions at lowest possible cost rather than optimizing information collection for decisions, and only discuss the latter case in Section 5.

Let us assume that we know the chosen quality of decisions to be achieved if uncertainty about each quality variable is below a given value $\sigma_{up}^{(j)}$. We shall denote the measurement schedule by a time-dependent vector $k(t) \in R^m$ the components of which are sums of delta functions at instants of measurements. The cost of measurement is denoted as *c(k(t))*. We allow the cost of measurement at a time instant to be a non-additive function of individual measurement costs but assume that the cost at one time instant does not depend on which measurements are made at other time instants.

In practise, measurements cannot be made at any time instant. For example, in papermaking the end product quality sample may be taken only when a machine reel has been completed, typically at 30 to 45 minutes intervals. Therefore, we consider a time-discretized scheduling problem, the discretization interval Δt being determined by the constraints set by the process or by other domain specific considerations. We also note that Mehra (1976) showed that the optimal schedule of scalar measurement can be constructed on measurements at most $m(m+1)/2+1$ instants, where m is the dimensionality of the state space. When time is discretized, the measurement vector $k(i)$ will be binary.

Let the optimization time horizon be $N\Delta t$ and let $0<\alpha<1$ be a discounting factor. Then the scheduling problem is formulated as

$$\begin{aligned}
&\min_{\{k(i)\}_{i=0}^{N-1}} \sum_{i=0}^{N-1} \alpha^{-i} c(k(i)) \\
&s.t. \\
&\Sigma(i+1) = \\
&\left(\left(\Sigma(i) + \left(\Sigma^{(ap)} - \Sigma(i) \right)\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D\Delta t \right)\right)\right)^{-1} + k(i+1)k(i+1)^T \otimes diag\left(\sigma_{meas}^{(j)^{-2}} \right)\right)^{-1} \\
&\Sigma(0) = \left(\Sigma_0^{-1} + k(0)k(0)^T \otimes diag\left(\sigma_{meas}^{(j)^{-2}} \right)\right)^{-1} \\
&\left(\Sigma(i) + \left(\Sigma^{(ap)} - \Sigma(i) \right)\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D\Delta t \right)\right)\right)_{jj} < \sigma_{up}^{(j)^2} \quad \forall j, \forall i = 0..N-1
\end{aligned} \qquad (11).$$

Here Σ_0 is the quality information covariance matrix before measurements at time $i=0$ are made. Symbol $\otimes$ denotes element-by-element multiplication of matrices.

The optimization problem (11) does not depend on which are the measurement values obtained. The solution will depend on the circumstances at the initial instant $t = 0$ only through Σ_0. However, if circumstances at $t = 0$ have arisen through similar optimization, then

$$\Sigma_0 \approx \Sigma^{(opt)}(N-1) + \left(\Sigma^{(ap)} - \Sigma^{(opt)}(N-1) \right)\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D\Delta t \right)\right) \qquad (12)$$

where $\Sigma^{(opt)}(i)$ refers to the covariance matrix under optimal policy. Note that exact equality cannot be achieved due to that measurement decisions are discrete.

Thus measurement scheduling is a policy optimization problem: it can be solved for once and all and then the resulting schedule applied cyclically. To solve for the policy two alternatives exist. Either one may choose the length of policy cycle N first, then add Eq. (12) to the constraints of (11) and solve the resulting optimization problem, or one may choose a large N in (11), solve without additional constraints and seek from the solution cyclic patterns after a transient period. In both cases discounting should be neglected by choosing $\alpha = 1$.

4. Solving the optimal schedule with simulated annealing

The measurement scheduling optimization of Eq. (11) is a complex integer programming problem. For example, if we have 10 measurements and 80 time intervals, the search space consists of 2^{800}, or roughly 10^{240}, solution candidates. We have chosen to solve the scheduling problem with simulated annealing (SA) that is rapid to implement and rather independent on the details of the problem. However, SA being a stochastic method does not guarantee global optimality of the solution found and may be in some cases rather slow. When applying SA we have followed the general guidelines in (Otten, van Ginneken, 1989).

SA requires a feasible solution as a starting point. Obviously, if all measurements are made at all time instants, the uncertainty in information about quality is minimized. Therefore, we use this point as the starting point of SA: if this is not a feasible solution, the set of feasible solutions is empty. The initial temperature is chosen to be 1.5 times the standard deviation of objective function of randomly chosen solution candidates, feasible or not feasible. Temperature scheduling is based on estimating global and local accessibility of the state space during the optimization. The Metropolis step is simply choosing a random instant and a random measurement and changing the corresponding binary value of k.

Let us consider an example of 5 measurements and 100 time intervals. In this example the *a priori* covariance matrix of quality parameters is

$$\Sigma^{(ap)} = \begin{bmatrix} 1.04 & 1.01 & 0.93 & 0.99 & 0.84 \\ 1.01 & 1.11 & 0.94 & 1.01 & 0.88 \\ 0.93 & 0.94 & 4.81 & 0.95 & 0.61 \\ 0.99 & 1.01 & 0.95 & 1.17 & 0.88 \\ 0.84 & 0.88 & 0.61 & 0.88 & 7.16 \end{bmatrix} \tag{13}$$

Therefore parameters 1, 2 and 4 are strongly correlated and their *a priori* variance is small, whereas parameters 3 and 5 are rather independent and with high *a priori* variance. Diffusion matrix is diagonal with 0.05 for each quality parameter and the time step $\Delta t = 1$. Measurement uncertainty of each measurement is $0.3^{1/2}$. Initial information matrix is diagonal with elements of 0.25 for each quality parameter.

Requirement on information uncertainty is specified as $\sigma_{up}^{(j)} = 0.3^{1/2}$. Cost of measurement is a mean value of two components: the number of parameters measured and a random component specific for each combination and distributed as Uni[0,1].

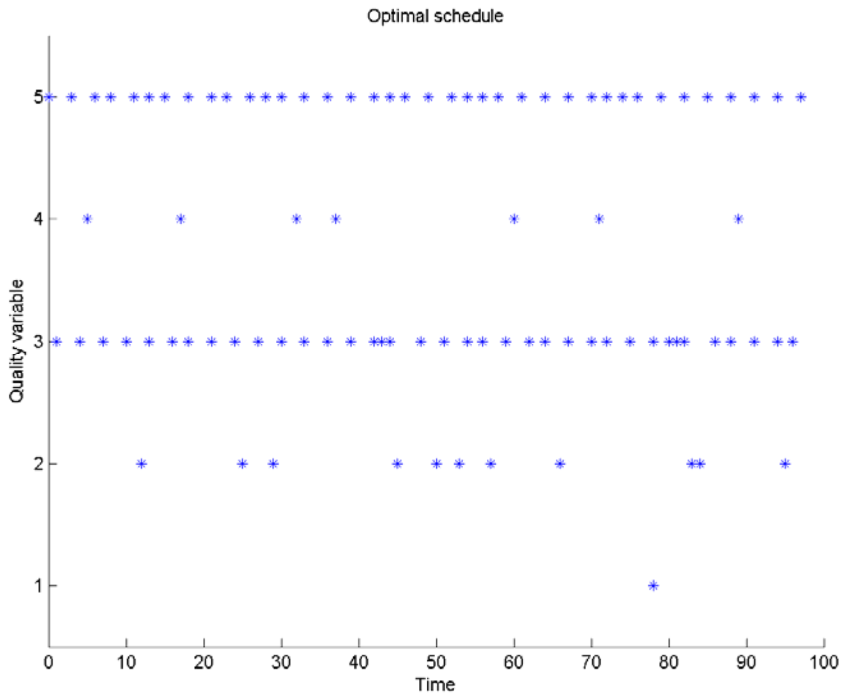

Figure 1. Example of an optimal schedule for 5 measurements over 100 time steps. Asterisk (*) denotes a measurement. Note that variables 2 and 8 are never measured but estimated on the basis of other measurements.

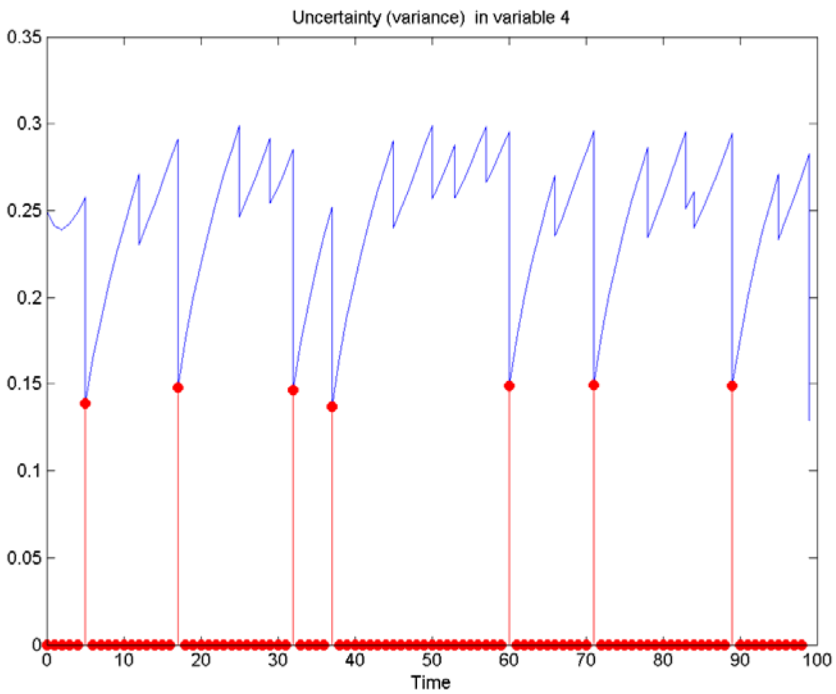

Figure 2. Predicted uncertainty in variable 4 corresponding to the optimal schedule in Figure 1. Red dots on curve denote instants for direct measurement of variable 4. Uncertainty (variance) is constrained to be below 0.3.

Figure 1 shows the optimal schedule. The optimization consisted of approximately 35000 feasible Metropolis steps in 98 temperature steps, and took some 20 minutes with Matlab and standard laptop. Towards the end of the optimization the fraction of feasible steps of all steps tends towards zero, and most of the optimization time was spent in the last 2000 feasible steps.

As expected by correlation structure quality variables 3 and 5 are frequently measured due to their high *a priori* variance and statistical independence. There appears no striking coherence between their measurement instants, which is due to that measuring them together represents a cost close to that of measuring them separately at different time instants. For quality variables 1, 2 and 4 measurements are less frequent due to more accurate *a priori* information and correlation between the variables. Figure 2 shows the variance in information about quality variable 4. The points with red dots indicate instants of actually measuring variable 4 whereas the other reductions in variance are due to measuring either quality variable 1 or 2. Note that quality variable 1 is measured only once over the optimization time horizon. This suggests that the optimal policy would entirely exclude measurement of variable 1.

The schedule in Figure 1 does not seem to converge to a simple cyclic policy. This is due to the rather special form of initial information covariance matrix and to that quality variables 3 and 5 are quite independent from the other variables – hence their measurement schedule is a policy that may be incommensurate with that of the other quality variables. Figure 3 shows another example of 80 time steps and 10 variables. In this case a convergence towards a cyclic policy is more apparent.

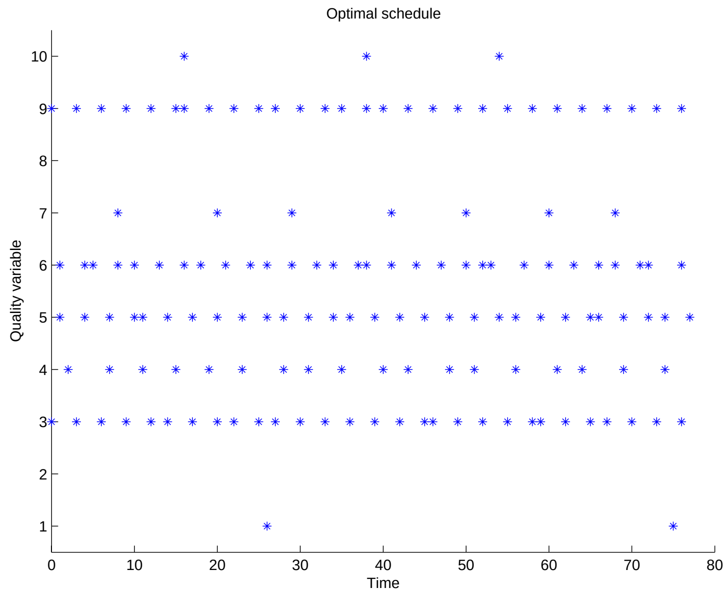

Figure 3. Example of an optimal schedule for 10 measurements over 80 time steps. Asterisk (*) denotes a measurement. Note that variables 2 and 8 are never measured but estimated on the basis of other measurements.

5. Discussion

Measurement scheduling is a two-goal optimization problem: minimize the costs and maximize the quality of information or quality of decisions. In the above we chose the cost to be optimized and quality of information to be constrained. Alternative formulation is to constrain costs and optimize the quality:

$$
\begin{aligned}
&\min_{\{k(i)\}_{i=0}^{N-1}} \sum_{i=0}^{N-1} \alpha^{-i} \sum_{j=1}^{m} \frac{\left(\Sigma(i) + \left(\Sigma^{(ap)} - \Sigma(i)\right)\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D\Delta t\right)\right)\right)_{jj}}{\sigma_{goal}^{(j)\,2}} \\
&s.t. \\
&\Sigma(i+1) = \\
&\left(\left(\Sigma(i) + \left(\Sigma^{(ap)} - \Sigma(i)\right)\left(1 - \exp\left(-\Sigma^{(ap)^{-1}} D\Delta t\right)\right)\right)^{-1} + k(i+1)k(i+1)^T \otimes diag\left(\sigma_{meas}^{(j)\,-2}\right)\right)^{-1} \\
&\Sigma(0) = \left(\Sigma_0^{-1} + k(0)k(0)^T \otimes diag\left(\sigma_{meas}^{(j)\,-2}\right)\right)^{-1} \\
&c(k(i)) < c_0 \quad \forall i = 0..N-1
\end{aligned}
\tag{14}
$$

The parameters $\sigma_{goal}^{(j)}$ define the relative uncertainty scale for quality variables and are thus similar in nature to $\sigma_{up}^{(j)}$ in formulation (11), except that one of them can be chosen arbitrarily due to that the scale of objective function does not affect the optimal schedule. The new parameter c_0 is the highest allowable cost of measurement per time unit. Solution of optimization problem (14) with industrial data has been discussed in Konkarikoski and Ritala (2006) and Gren et al (2007a, 2007b).

Solution of problem (14) does allow uncertainty in some of quality parameters at some time instants to be rather high through compensation of very low uncertainty in other parameters/time instants. Typically, this is not preferable for decision making. However, a common practical case is that a number of measurements, n_{meas}, can be made with normal resources and exceeding this number will involve additional people and/or equipment. This corresponds to that the cost of measurement *c(k)* is a function of only on the number of measurements made and that it is an abrupt function at n_{meas}. In such cases formulation (14) is preferred to that of (11).

In practical implementations finding the uncertainty constraint, respective scaling parameters, for formulations is the main difficulty. At paper mills where the scheduling has been tested no process engineers or operators have been able to answer directly questions, such as “what is allowable uncertainty about paper strength”. Instead, defining the uncertainty constraints must be based on detailed analysis on how quality information is utilized when process and quality management actions are decided upon. In particular, the uncertainty constraints should not be set up on the basis of measurement accuracy: some of the quality parameters are actually measured with accuracy far better than needed in decision making whereas others can barely be measured with the accuracy required for decisions.

An additional degree of freedom in measurement scheduling is to make several measurements on a quality variable. This is easily incorporated to the formulations (11) and (14) by allowing k to take values $n_r^{1/2}$, where $n_r = 0, 1, 2\ldots$ is the number of independent repeats rather than binary values only. However, this enlarges the search space from $(2m)^N$ to $((n_{r,max}+1)m)^N$, where $n_{r,max}$ is the maximum number of repeats.

Ideally, measurement scheduling should be linked directly to decision optimization so that measurement selection is part of the action space. Meier at al (1967) discussed such control problems from dynamic programming point of view. In particular, they showed that for linear systems, quadratic cost, and Gaussian stochastic effects, the decision optimization can be carried out independently on measurement scheduling optimization, and that measurement scheduling reduces to a regular cyclic policy optimization. However, quality information is utilized in practice to rather intuitive and unstructured decision tasks, and even when the decision tasks have been formulated as optimization problems, they tend to be rather complex to solve. Thus establishing the direct link between measurement scheduling and decision making about quality has turned out extremely difficult. This led us to separate the two problems by formulations (11) or (14) at the expense of specifying the uncertainty constraint, respective scaling parameters.

6. Conclusions

Current industrial practice for scheduling measurements has evolved gradually over a long period of time and without systematic analysis. Our experiences show that a considerable amount of resources is allocated to collecting information rather useless for operation at the expense of neglecting acquisition of some operationally critical quality information. Therefore an urgent and practical need for optimizing the scheduling and the extent of off-line quality information exists.

In this presentation we have outlined the foundation for practical measurement scheduling to support quality and process management in process industries, such as the papermaking industry. This approach relies heavily on ideas presented more than three decades ago by Mehra (1976), and even earlier by Meier et al (1967), but which have been little used in quality management of process industries.

The measurement scheduling presented here is systematic once the uncertainty constraint, respective scaling parameters have been determined. However, these parameters can be determined only through a rather tedious analysis of how quality information is utilized in operational decisions. We suggested and will continue our work towards integrating the optimization of operational actions and measurement collection. As many operational decisions are made intuitively rather than by structuring them into decision optimization problems and the solving them, also this approach must be supported with detailed analysis on operational decision making. Simple examples of such operational decision analyses in papermaking industry are given e.g. in Jokinen et al (2006).

Acknowledgements

This work has been supported in part by Finnish Agency of Technology and Innovation (TEKES) through project “Production 2010” and partly through Academy of Finland through project “Systematic design of measurement systems, SyDeMIS”.

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