Cautious On-Line Correction of Batch Process Operation

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Most industrial batch processes are operated through open-loop application of an off-line optimized input profile, such as feed or temperature. This is because modeling accuracy is typically poor (Juba and Hamer, 1986), and direct concentration measurements that would allow to cope with the frequently encountered lack of reproducibility are rare.

However, when on-line measurement information gives access to the system state, on-line reoptimization promises considerable improvement. Since industrial on-line measurements typically do not immediately reveal perfect information on the entire system state, on-line state and parameter estimators need to be used. Their estimates often contain non-negligible uncertainty due to the system state being inferred from indirect, so-called model-based measurements, which can be subject to both stochastic measurement noise and structural measurement-model mismatch.

Given such estimates, it is common practice to perform on-line optimization ignoring their uncertainty. Still, this is optimal theoretically only for ideal linear systems rather than possibly strongly nonlinear batch processes. Another approach is to begin with the open-loop optimal profile and switch to on-line optimization either empirically after a given number of measurements or when estimate uncertainty is sufficiently small. This leaves the problem of finding a good compromise between waiting for good estimates and reacting sufficiently early, as sensitivity of the final operation objective to input changes usually decreases rapidly.

The present contribution suggests a cautious on-line correction mechanism that replaces the switching from open-loop to closed-loop operation with a smooth transition controlled by estimate uncertainty. Its single scalar tuning parameter represents the desired degree of cautiousness or boldness with which current estimates are used for on-line correction of open-loop optimized input profiles. In the limiting cases of no information (large uncertainty) and perfect information (certainty), the corrector naturally reduces to optimal open-loop and optimal feedback operation, respectively.

Cautious Correction and Interpolation

Single profile correction

Given a state estimate $\hat{x}$ and an estimate of its variance/covariance matrix P_x from a state estimator, such as the extended Kalman filter (EKF) (Jazwinski, 1970), the $\Delta\chi^2$-test (Bard, 1974) can be used to check whether or not a point x of the state space lies in a linearized γ %-confidence region of the estimate. For a model with p degrees of freedom, such a point does lie in this region if (and only if) it satisfies the inequality:

$$(x-\hat{x})^T P_x^{-1}(x-\hat{x}) \leq \Delta\chi^2(\gamma, p) \tag{1}$$

where $\Delta\chi^2$ can be taken from statistics tables or can be computed from the Γ function.

Given an open-loop optimal trajectory for control $u^*(t)$ and state $x^*(t)$, Eq. 1 could in principle be used as a criterion for switching from the open-loop optimal $u^*(t)$ to an on-line optimized $u(\hat{x})$. As the exact reoptimization is normally too demanding to be performed on-line, state feedback remains the more feasible alternative. Different approaches to optimizing state feedback can be found in Palanki et al. (1993) (singular), (Terwiesch and Agarwal, 1994) (nonsingular) and (Cuthrell and Biegler, 1989) (reoptimization).

In order to eliminate undesirable side effects of binary switching between open-loop and feedback operation such as oscillation between the two, a smooth transition is sought to replace switching based on Eq. 1. Even states that lie several standard deviations away from their nominal value should only influence the decision about the correction if they have an impact on the optimal control.

Consider the following definition of a cautiousness factor:

$$\mathcal{C} \triangleq 1 - e^{-\alpha(K\delta\hat{x})^T(KP_xK^T)^{-1}(K\delta\hat{x})} \tag{2}$$

where $K = \partial u/\partial x$, $\delta\hat{x} = \hat{x} - x^*$ and α is a scalar tuning parameter. In the general transition scheme:

$$u = (1-\mathcal{C})u^*(t) + \mathcal{C}u(\hat{\mathbf{x}}) \tag{3}$$

that gradually shifts between off-line optimized $u^*(t)$ and on-line estimate-based $u(\hat{x})$, a smaller value of α leads to a smaller value of $\mathcal{C}$, thus causing the controller to stick more cautiously to the open-loop policy rather than rely on current state estimates for correction, as would be the case for larger values of α. In the limiting cases of perfect information (P_x

$\rightarrow 0$) and no information ($P_x \rightarrow \infty$), the controller naturally reduces to optimal feedback control and optimal open-loop operation, respectively. The scalar tuning parameter α can be used to adjust the desired level of conservativeness/boldness in using the current estimates for endpoint optimizing feedback. The extreme setting $\alpha \rightarrow 0$ is equivalent to total disbelief in the estimates and thus leads to optimal open-loop control, while large tunings $\alpha \rightarrow \infty$ cause the corrector to entirely believe the estimates and ignore their uncertainty.

Note that the definition of Eq. 2 is independent of numerical scaling of x and u coordinates, and that $P_u \triangleq KP_xK^T$ can be interpreted as the covariance of the correction $\delta\hat{u} = u(\hat{x}) - u^*(t)$. For infinitesimal changes, the term $\delta\hat{u}^T P_u^{-1} \delta\hat{u}$ can be understood as the square of the *generalized distance* in coordinates of the estimate variance and is a measure of significance of the projected control change $\delta\hat{u}$ given an estimate $\hat{x}$, its variance P_x, and a control law $u(\hat{x})$. It remains small, and $\mathcal{C} \rightarrow 0$, when $\hat{x}$ and x^* are not significantly different or when $\partial u/\partial x$ is small in the direction of their distance, and is large, and $\mathcal{C} \rightarrow 1$, as $\delta\hat{x}$ becomes significant in view of the variance/covariance P_x amplified by the gain $\partial u/\partial x$. (See section 4, Figure 5, for an illustrative example.)

For example, a cautious form of the neighboring extremals correction $\delta\hat{u}(t) = K(t)\delta\hat{x}(t)$ investigated for the case of perfect state estimates in (Terwiesch and Agarwal, 1994) is:

$$u(t) = u^*(t) + \mathcal{C}K(t)\delta\hat{x}(t) \tag{4}$$

Here, the optimal linear time-variant correction gain $K(t)$ can be precomputed off-line through backwards integration of a matrix Riccati type ODE around the optimal ($x^*(t)$, $u^*(t)$), thus reducing the on-line computing effort of the optimization part to that of a P-controller. Application of the cautious optimizing state feedback (Eq. 4) will be demonstrated on a numerical example in the third section. However, the cautious transition scheme (Eqs. 2 and 3) is more general and can also be used with the other types of on-line optimization discussed above. Note that generalization to the case of multiple nominal trajectories is straightforward and allows to cover larger regions of uncertainty.

Simulation Example

Process model and objective

Consider the following series reaction conducted in a nonisothermal batch reactor:

$$2A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

The reaction kinetics, a second order decomposition followed by an autocatalytic one, can be described by

$$\frac{d}{dt}[A] = -2k_1[A]^2$$

$$\frac{d}{dt}[B] = k_1[A]^2 - k_2[B][C]$$

Temperature dependence follows the Arrhenius' law:

$$k_i(T) = k_{i,0}e^{-\frac{E_i}{RT}}, \quad i \in [1, 2]$$

where $k_{1,0} = 80$, $k_{2,0} = 600$, $E_1 = 22$, and $E_2 = 33$. Initially the reactor is filled with A, contaminated with a small amount of C, and no B is present. The objective of the optimization is to determine the temperature profile $T(t) \in [290, 420]$ that, for the given batch time $t_f = 1$, maximizes the ratio J of the desired B to the undesired A and C:

$$\max_{T(t)} \left. \frac{[B]}{[A]+[C]} \right|_{t=t_f}$$

This objective strives simultaneously for a high B production and a low burden of subsequently separating A and C from the desired product.

Estimation

Given simulated measurements of heat generation y_1 (inferred from temperature measurements) and of absorbance y_2 at a specific wavelength:

$$y_1 = k_1[A]^2 \Delta H_{r1} + k_2[B][C]\Delta H_{r2}$$

$$y_2 = c_1[A] + c_2[B] + c_3[C]$$

the three concentrations and the rate constant factor $k_{1,0}$ are estimated on-line using an EKF. Since both measurements are corrupted with noise (see Figure 1), the filter yields estimates with nonnegligible variance, especially for $[C]$. While the filter starts from the nominal $[\hat{A}]_0 = 0.996$, $[\hat{B}]_0 = 0$, $[\hat{C}]_0 = 0.002$, $\hat{k}_{1,0} = 80$, which are also the nominal values for which the optimization is performed, the true process is simulated with $[A]_0 = 0.992$, $[B]_0 = 0$, $[C]_0 = 0.004$, and $k_{1,0} = 144$, meaning that both reaction steps proceed more quickly than nominal. For a typical profile of the states and their estimates, see Figure 2. (Numerical values: $c_1 = 1$, $c_2 = 1$, $c_3 = 5$, $\Delta H_{r1} = 0.2$, $\Delta H_{r2} = 0.5$.)

Results

The present section summarizes results obtained in comparison of cautious correction against estimate feedback and open-loop operation. The cautious feedback (4) includes the concentration states and the estimated rate constant factor $\hat{k}_{1,0}$, which is readily incorporated into the neighboring extremals framework.

Figure 3 compares temperature profiles for cautious ($\alpha = 0.5$) and noncautious correction and open-loop operation for

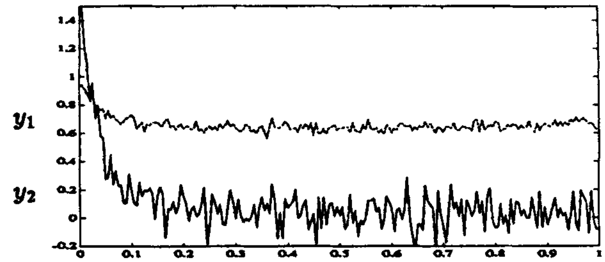

Figure 1. Measurements.

—— y_1, - - - y_2.

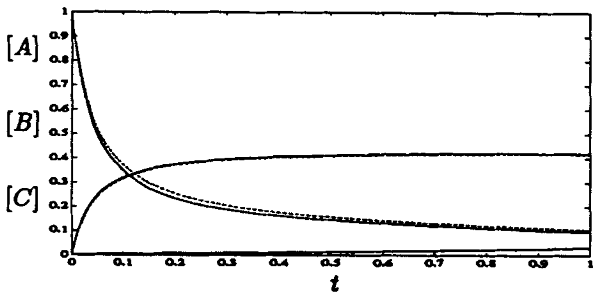

Figure 2. Concentration.

—— true; - - - estimated.

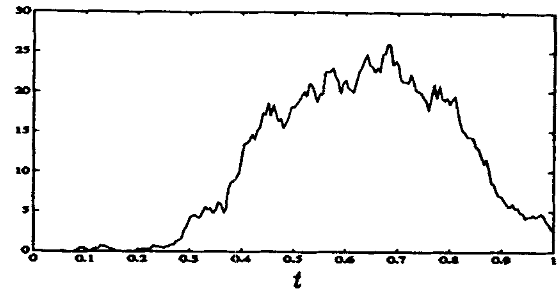

Figure 4. Significance $\delta\hat{u}^T P_u^{-1}\,\delta\hat{u}$.

the same run as above. While both corrected profiles achieve substantial performance improvement relative to open-loop operation, the estimate feedback starts correcting in the wrong direction initially.

For the same run, Figure 4 shows the evolution over time of the significance measure $\delta\hat{u}^T P_u^{-1}\delta\hat{u}$. The EKF is able to estimate the off-nominal value $k_{1,0}$ comparatively well from the first few data points due to the strong initial heat generation. However, the significance measure $\delta\hat{u}^T P_u^{-1}\delta\hat{u}$ remains small until $t \approx 0.3$, as not enough information regarding $[C]$, to which the optimal strategy is most sensitive, is available before.

A similar situation is illustrated in Figure 5, where the current estimate $\hat{x}$, '×', and its 90% confidence ellipse for known $k_{1,0}$ are shown in the $[A]$, $[B]$ plane together with lines of constant u (solid). Separate information on $[C]$ is obviated through mass balance. While $\hat{x}$ is significantly different from the precomputed nominal x^*, '∗', its projection on the control gradient is small (2 units) relative to that of the confidence region. In comparison, for a hypothetical nominal $\tilde{x}$, '○', that still lies within the confidence region, this projection would be considerably larger (5 units), thus calling for stronger correction.

Figure 6 shows performance J of cautious (solid) and estimate feedback (dashed) relative to open-loop performance J_{nom} for a range of cases with $[C]_0$ mismatch and no $k_{1,0}$ mismatch. In the vicinity of the nominal value $[C]_0 = 0.002$ (dotted), estimate feedback performs worse than open-loop operation, while the cautious feedback practically retains open-loop optimality. In the case of far less $[C]_0$ than nominal, estimate feedback performance is superior, as it creates a strong response based on the first few measurements, while the cautious corrector is hesitant to take any other decision than the nominal policy since no clear information regarding even the sign of the optimal correction is available. This attitude pays in the opposite case, when more $[C]$ is present initially, as the estimate feedback similarly to Figure 3 first corrects in the wrong direction while the cautious feedback still sticks to the open-loop policy and waits for statistically more significant information. Considering the results obtained for the whole range of simulated mismatches, especially when weighted by a probability distribution that has its mean at the nominal value, the cautious corrector's overall performance is visibly better than that of direct estimate feedback.

Changing the coefficients of the second measurement equation to $c_1 = 1$, $c_2 = c_3 = 2$ produces constant absorbance for all times and makes any $[C]_0$ mismatch unobservable. While an estimate-based mechanism would still attempt to correct the temperature profile, the cautious corrector sticks to the open-loop policy, since it automatically 'notices' the lack of measurement information that could be used for correction.

Discussion

While the considerations leading to the formulation of the cautious corrector are of a statistical nature, no claim regarding theoretical optimality of the proposed approach, especially the empirical definitions (Eqs. 2 and 3) is made.

Also, the author freely admits that the present work depends on the availability of realistic estimates not only of the system states but also of their variances. The latter are not always available, since especially in cases with many data points and small measurement noise the EKF tends to underestimate the state variance (Jazwinski, 1970). However,

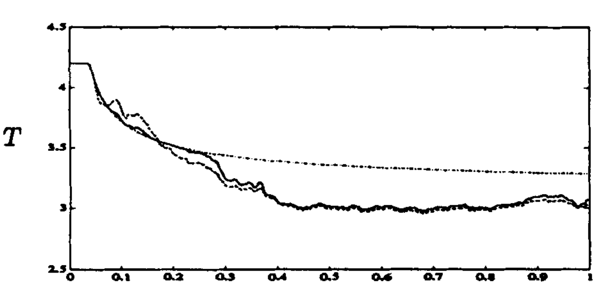

Figure 3. Temperature profiles.

—— cautious; - - - estimate feedback; · — · — open loop.

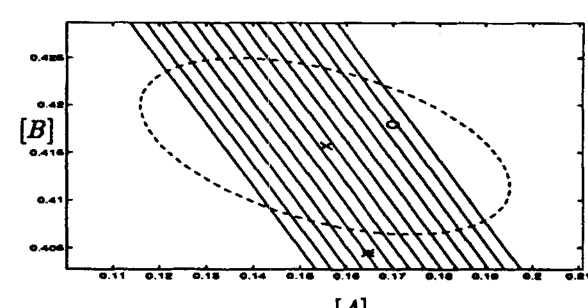

Figure 5. Estimate with confidence ellipse.

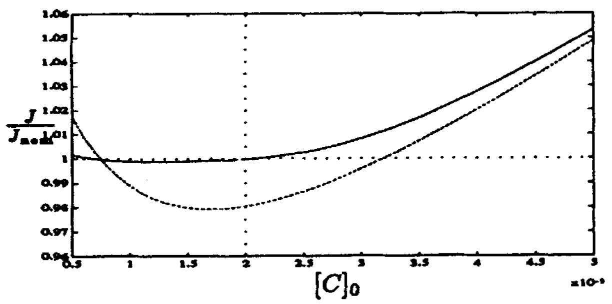

Figure 6. Performance comparison.
—— cautious; - - - estimate feedback.

this is typically more a problem of continuous rather than batch processes and can be resolved by replacing the EKF with a computationally more expensive estimator based on the method of sensitivity equations (Bard, 1974). Even when an insufficient number of computing resources for on-line implementation of such an improved estimator are available, it can be used off-line as a reference for appropriately tuning the EKF.

The choice of tuning parameter α is comparatively straightforward, since the interpretation of Eq. 2 as a mapping from $\Delta\chi^2$ to $\mathcal{C} \in [0, 1]$ allows the effect of the tuning to be relatively well anticipated as values of $\Delta\chi^2$ are known given the number of degrees of freedom p and a desired confidence γ.

An open problem is that estimate feedback often produces relatively 'nervous' controls that may be unsuitable for practical implementation, and that the cautious corrector inherits this undesirable property when estimates are several standard deviations from nominal. While the most rigorous approach would be to incorporate control smoothing into the on-line optimization, such as by penalizing large control changes, a shortcut adjustment can be made by increasing the measurement noise covariance $\boldsymbol{R}$ in the tuning of the EKF.

Conclusion

A cautious corrector that incorporates uncertainty of state estimates into on-line batch optimization has been presented and subsequently demonstrated on a simulation example.

A single scalar tuning parameter is used for user specification of a desired degree of cautiousness or boldness in believing current estimates and their variances for on-line correction or reoptimization of open-loop optimized input profiles. In the limiting cases of no information and perfect information, the corrector reduces to optimal open-loop and optimal feedback operation, respectively.

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