Monitoring and improving LP optimization with uncertain parameters

Danielle Zyngier*, Thomas E. Marlin

Dept of Chem Eng, McMaster Univ, 1280 Main St. W, Hamilton, ON, L8S4L7, Canada

Abstract

Linear Programming (LP) remains the workhorse of applied optimization, having open-loop process applications such as production planning, inventory scheduling and closed-loop applications such as Real-time optimization and the steady-state determination at each execution of a Model Predictive Controller (MPC). This paper presents new methods for monitoring performance (estimating the degradation due to uncertainty) and for improvement (reducing the uncertainty, when required, through economically optimal experiments) of closed-loop RTO systems.

Keywords: RTO, performance monitoring, LP, uncertainty, experimental design

1. Introduction

The value of optimization in plant operating planning and scheduling is well recognized. Potentially large benefits are possible when the optimum operation point changes often, i.e., there are significant disturbances in the process or changes in economics (Marlin and Hrymak, 1997; White, 1997).

Little research has investigated monitoring, diagnosing and improving the performance of closed-loop economic optimization. In this paper, a systematic procedure is presented that is not limited to a constant active set, provides a measure of economic degradation due to model errors, identifies key parameters for a scenario, and designs plant experiments for improved model accuracy giving better economics performance.

This paper investigates a real-time optimization (RTO) system with an LP optimizer with feedback information compensating for disturbances. The method is presented and applied to a case study involving blending gasoline in a petroleum refinery. In this example, five components (Reformate, LSR Naphtha, n-Butane, FCC Gasoline and Alkylate) are blended into the final gasoline product. The quality measurements in this system are the product blend octane and Reid vapour pressure (RVP) that are measured frequently onstream. The uncertainty in the case study lies only in the octane and RVP properties of the feed components to the blend, which are not measured due to the high cost of analyzers. Also, closed-loop simulations include measurement errors typical for industrial systems. A linear blending model was achieved through the use of blending indices (Gary and Handwerk, 1984) and the use of “blend-quality” inequality constraints (Pedersen et al., 1995).

The closed-loop RTO solves Eq.(1) at each execution, which is equivalent to industrial blending optimization systems (Pedersen et.al., 1995). In Eq. (1), $F_i$ represents the flow of each feed component, $value$ is the value of product gasoline, $cost_i$ is the cost of each component, $Q_{ij}$ represents the qualities of each component in the model and the subscript blend refers to the final blended gasoline. The feedback bias terms $\epsilon$ for octane

* Current address: Honeywell Process Solutions, 300 Yorkland Blvd., M2J 1S1, Toronto, Canada.
and RVP are calculated before the optimization problem as the difference between the predicted and measured quality (as in an MPC) and are, therefore, constants in Eq. (1).

\[
\begin{align*}
\text{max} & \sum_{i} (\text{value} - \text{cost}) F_i \\
\text{s.t.} & \quad Q^j_{\text{blend, min}} \leq \sum_{i} F_i (Q^j_{i, \text{model}} + \epsilon^j) \leq Q^j_{\text{blend, max}} \sum_{i} F_i \\
\text{Demand}_{\text{min}} & \leq \sum_{i} F_i \leq \text{Demand}_{\text{max}} \\
& \quad 0 \leq F_i \leq \text{Available}_i
\end{align*}
\]

2. Five-Step Monitoring and Enhancement Procedure

**Step 1: Data Rectification:** The first step consists of checking the data for consistency with the model and the uncertainty description. This step is needed because the subsequent steps rely on a priori estimates. If these are in error, the user should problem-shoot a major fault in the plant before implementing RTO. This step uses published methods (e.g., Johnston and Kramer, 1995).

**Step 2: Evaluating CLRTO Performance:** The next step is to determine whether model/plant mismatch could lead to a significant profit loss; if a significant loss is possible, we will reduce the mismatch in subsequent steps. The potential loss due to parameter mismatch is the difference (gap) between the "ideal case" (CLRTO with no parameter mismatch) and "actual case" (CLRTO with parameter mismatch). The “worst-case” scenario, leading to the largest profit loss, occurs when the component qualities (within their uncertainty bounds) maximize the profit difference. In Step 2, the maximum profit loss, or the maximum improvement, is evaluated by finding the scenario of component qualities that maximize the profit gap.

This approach is formulated as the following bilevel programming problem.

\[
\begin{align*}
\text{max} & \quad \sum_{i} (\text{value} - \text{cost}) F_i \\
\text{s.t.} & \quad \text{max}_{F_i} \quad \text{Pr}_{\text{RC}} = \sum_{i} (\text{value} - \text{cost}) F_i \\
& \quad \text{max}_{F_i} \quad \text{Pr}_{\text{WC}} = \sum_{i} (\text{value} - \text{cost}) F_i \\
& \quad \sum_{i} F_i (Q^j_{i, \text{model}} + \epsilon^j) = Q^j_{\text{blend, max}} \sum_{i} F_i \\
& \quad \sum_{i} F_i (Q^j_{i, \text{model}} + \epsilon^j) = Q^j_{\text{blend, max}} \sum_{i} F_i \\
& \quad \text{Demand}_{\text{min}} \leq \sum_{i} F_i \leq \text{Demand}_{\text{max}} \\
& \quad 0 \leq F_i \leq \text{Available}_i
\end{align*}
\]

In this problem, the inner optimization problems \(\text{Pr}_{\text{RC}}\) and \(\text{Pr}_{\text{WC}}\) determine the values of the flowrates that yield the maximum profit, while the outer level determines the values of plant component quality parameters that maximize the profit gap. The “worst-case” sub-problem \(\text{Pr}_{\text{WC}}\) takes feedback into account because final closed-loop steady state profit is considered. Since the “best-case” sub-problem \(\text{Pr}_{\text{RC}}\) considers a perfect model, feedback is not needed, so a simpler formulation is possible.

To facilitate the solution of Eq. (2), the two inner optimization problems are replaced with their Karush-Kuhn-Tucker optimality conditions (Clark and Westerberg, 1990). For the blending case study in this work, the bilevel programming problem
consisted of 56 variables (due to the inclusion of Lagrange multipliers) and 44 complementarity constraints arising from the optimality conditions of the inequality constraints. In our experience, local optimal solutions were obtained very reliably by using IPOPT-C, an interior point solver tailored to handle complementarity constraints (Raghunathan and Biegler, 2003). Problems converged quickly ($< 2.0$ CPU seconds) to local solutions for the case studied in this paper. It is worth mentioning that even though this is a non-convex optimization problem, several starting conditions converged to the same optimum point, building confidence in the results.

**Step 3: Updating Parameters Using CLRTO Data:** If the profit gap evaluated in Step 2 is deemed significant (say over $100$ per day), we would like to reduce model mismatch by using available measurements to estimate the uncertain parameters. The parameter-updating strategy used here is Bayesian Estimation, which allows for the incorporation of prior estimates of the parameter uncertainty and prevents unnecessarily large plant experiments (Box and Tiao, 1973). The estimated parameter values are obtained by using the following equation (Reilly, 1973).

\[
Q_t = (\text{Var}(Q)|_{t-1} + X^T \text{Var}(z)^{-1} X)^{-1} (\text{Var}(Q)|_{t-1} + X^T \text{Var}(z)^{-1} z)
\]

(3)

In Eq.(3), \(\text{Var}(Q)|_{t-1}\) is the prior variance-covariance matrix of the parameters, \(Q_t\) and \(Q_{t-1}\) are the matrices with the new and initial parameter estimates, \(X\) is the matrix with input variables and \(\text{Var}(z)\) is the variance-covariance matrix of the output variables (measurements). In the case study, the output variables \((z)\) considered were blend octane and RVP properties. When using the estimation method in Eq. (3), the parameter uncertainty can be shown to decrease with the experiments according to the following equation (Reilly, 1973).

\[
\text{Var}(Q)|_t = (\text{Var}(Q)|_{t-1} + X^T \text{Var}(z)^{-1} z)^{-1}
\]

(4)

Since the RTO introduces changes to manipulated variable values in response to model error and disturbances, initial closed-loop data from the current batch) is available at no cost and might have information useful in estimating RTO model parameters. Although this is a feedback system without external perturbations, Eq. (3) can be applied because of the lack of disturbances in the component qualities leaving large storage tanks.

**Step 4: Designing Profit-Based Experiments:** If Step 3 does not reduce the potential loss below the threshold, designed experiments can be performed on the plant. The experimental design formulation is presented in the following. The variables being adjusted by the outermost problem are the component flowrates during the experiment; however, feedback information can be used by including the updated bias information \((\epsilon)\) in the experimental design calculation. This data at new
operating conditions affect $\text{Var}(Q_{\text{plant}})$ through $X_{\text{exp}}$, thus reducing the uncertainty region, i.e., tightening the upper and lower bounds of the $\text{MaxPrGap}$ sub-problem in Eq. (2).

The key issue in proposed experimental design strategy is the trade-off between the cost of experimenting and the benefits of an improved model in the closed-loop system, represented by the objective function in Eq. (5). In order to quantify this trade-off in terms of profit, a measure of time is needed. Since the case study in this work is a batch process, $t_1$ the time remaining (days) in the batch after experimentation, while $t_2$ is the time needed (days) to perform the experiment.

The formulation in Eq. (5) is a three-level optimization problem, which was solved by using an unconstrained direct search method known as Derivative-Free Optimization (DFO) (Conn et al., 1997). The constraints (5c)-(5f) were replaced by penalty terms in the objective function in Eq. (5). DFO is based on approximating the objective function by a (simpler) surrogate model within a trust region, and then optimizing the surrogate model to obtain an improved point. It has been shown to be globally convergent to a local solution, and to be computationally more efficient than other direct search methods (Wright, 1996). For these reasons, the Matlab implementation of the DFO algorithm developed by Fan (2002) was used.

**Step 5: Implementing New Values:** The new parameter values are inserted in the CLRTO model.

### 3. Results

The five-step procedure was applied to a gasoline-blending system. The process was assumed to have independent initial uncertainties for octane and RVP properties in the 5 components ($\pm 0.47$ octane numbers or psi). Measurement errors were assumed to be $\pm 0.2$ octane numbers and $\pm 0.15$ psi for octane and RVP qualities of the final blend, respectively, and 0.5% of the actual rate for flow measurements. These are realistic estimates of the uncertainties encountered in industrial gasoline-blending processes (Szoke and Kennedy, 1984). No gross errors were included in the simulated measurements.

The five-step diagnostic procedure was initiated when the blend and real-time optimization began. After 4 RTO runs, the process under closed-loop RTO was achieved steady-state operation with a profit of $8,549/day. The component flowrates can be seen in Fig. (1).

![Component Flowrates during Case Study](image-url)
**Step 1 – Data Rectification:** According to the chi-square test, the data remained within the expected uncertainty.

**Step 2 – Evaluating CLRTO Performance:** Eq. (2) indicated that the “best-case” scenario ($Pr_{BC}$) was $9,810.3/day, while the “worst-case” scenario ($Pr_{WC}$) was $7,604.9/day. This yielded a profit gap of $2,205.4/day, which was deemed too large.

**Step 3 – Updating Parameters Using CLRTO Data:** Data from the first three CLRTO iterations was used to update parameters using the Bayesian Estimation method in Eqs. (3) and (4). After this was done, the largest profit gap in Eq. (2) was equal to $1,785.6/day, which was still considered too large.

**Step 4 – Designing Profit-Based Experiments:** Assuming a blend with 9 hours of operation remaining, and a 15-minute long experiment, the weightings $t_1$ and $t_2$ used were 0.3646 day and 0.0104 day, respectively. After designing seven profit-based experiments (one at a time) according to Eq. (5), the largest profit gap calculated using Eq. (2) was reduced to $82.1/day.

**Step 5 – Implementing New Values:** After applying the improved parameter estimates obtained in Step 4 in the CLRTO model and returning the CLRTO to closed-loop operation, the system converged to a new operating point with Reformate, LSR Naphtha and n-Butane being blended to produce gasoline. This new operation yielded a profit of $9,118.1/day. It is important to note that the gasoline blend resulting from the two different operation points (the initial and the final ones in Fig. (1)) both produced gasoline with their maximum RVP and minimum octane, which is expected from an efficient gasoline-blending process (Gary and Handwerk, 1984). The difference between the operating strategies lies in the use of less expensive components in the more profitable operating strategy to achieve the same blend qualities. Assuming a single gasoline-blending batch per day, the benefits obtained from applying the procedure to this case study would be of approximately $208,000/year increased profit over a current state-of-the-art industrial blend optimization system.

### 3.1. Case with Different Economics (Case 2)

Given the same initial RTO model/plant parameter mismatch as in the previous case study (Case 1) but different economic parameters in Cases 1 and 2, the initial operation of the CLRTO yielded the same initial optimal basis as in the preceding case, with LSR Naphtha, n-Butane and Alkylate being blended. The final uncertainties that result from the application of the 5-step procedure to each case after 10 designed experiments can be seen in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Octane uncertainty (octane)</td>
<td>RVP uncertainty (psi)</td>
</tr>
<tr>
<td>Reformate</td>
<td>±0.11</td>
<td>±0.08</td>
</tr>
<tr>
<td>LSR Naphtha</td>
<td>±0.37</td>
<td>±0.33</td>
</tr>
<tr>
<td>n-Butane</td>
<td>±0.46</td>
<td>±0.45</td>
</tr>
<tr>
<td>FCC Gas</td>
<td>±0.47</td>
<td>±0.46</td>
</tr>
<tr>
<td>Alkylate</td>
<td>±0.15</td>
<td>±0.12</td>
</tr>
</tbody>
</table>

Table 1. Parameter Uncertainty after Experimentation

In Case 1, the key decision is between Reformate and Alkylate; in Case 2, the key decision is between FCC gasoline and Alkylate. This case study demonstrates that the
A five-step procedure is able to identify the key model parameters for the specific scenario and to reduce the uncertainty in the key parameters with economically optimal plant experiments. These important features are achieved without guidance from the user.

4. Conclusions

A sequential five-step method to monitor and enhance the performance of closed-loop RTO systems has been developed in this work. This procedure provides quantitative measure of potential improvement. Since the true plant is not known, the method determines the largest gap between the best- and worst-case profit scenarios due to parameter variation within their uncertainty region.

In addition, the method reduces uncertainty to increase profit with the least disruptive experiments possible. In order to reduce the severity and number of plant experiments needed in the five-step procedure, prior knowledge about the parameter distribution is considered when estimating model parameters by using Bayesian estimation. A new cost-effective experimental design strategy was proposed. It considers the trade-off between improving the closed-loop RTO model and the cost of performing the experiment. Besides being performed under the most profitable conditions possible, the experiment also obeys process constraints.

This work adds to the current state-of-the-art in monitoring optimization performance. It is not limited to a single active set, can handle open or closed-loop systems, addresses correlated parameter uncertainty, emphasizes the objective value (rather than a measure or information), and provides a new experimental design method. Future extensions include applications for sensor selection to reduce experimentation, at the cost of capital equipment.

References