**Machine Learning in the context of the Modifier Adaptation Methodology for Real Time Optimization.**

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**Highlights**

* Machine learning implemented in the modifier adaptation method.
* Rejection of disturbances and modelling mismatch in real time optimization.
* Method allows tracking the optimum of an uncertain process in spite of disturbances.

**1. Introduction**

Real Time Optimization (RTO) with Modifier Adaptation method (MA) allows finding the optimum of a process () when the model of the process presents structural mismatch. To do so, MA updates the decision variables (), solving iteratively a modified model-based optimization problem, updated with first ()and zeroth () order corrections in the objective function () and in the inequality constraints (). are calculated using process gradients with respect to [1]. As the process is uncertain, the experimental gradients are calculated with historical data. In real processes unmeasured disturbances () can affect the process outputs, i.e. and. Therefore, the process derivatives calculated only with past information of can be erroneous, which implies that the MA may not find [2]. To avoid the estimation of the process gradients, MA has been reformulated as a nested optimization problem (NMA) [3]. NMA uses an upper optimization layer to update , looking for the minimization of the Lagrangean of the process (). As can affect the outputs, it is expectable that **.** Machine Learning (ML) is a subset of artificial intelligence algorithms that uses statistical techniques to give computers the ability to learn with data. It allows overcoming the uncertainty related with the modeling-mismatch of a process building internal surrogated models based in statistical analysis. It relays in the idea of sequential queries to the real process, each of them calculated solving an optimization problem with the surrogated model. At each evaluation in the process, the model uses the gathered data to increase the knowledge of the uncertain system. The objective of this work is the implementation of algorithms based in ML in the upper layer of NMA (ML-NMA) to give the MA the ability to track the value of in real time.

**2. Methods**

For a given steady state , the upper layer proposes solving Eq.(1), where is the available mapping of . is obtained with the Gaussian Process approach (GP). GP is a nonparametric regression method to find an approximation of with the available data.

|  |  |
| --- | --- |
|   | (1) |

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Lower Layer and Process

ML-based upper layer Eq.(1)

Modified optimization Eq. (2)

0th order corrections

**Figure 1.** Developed algorithm of NMA with ML (ML-NMA).

The value of and , are used to solve the modified optimization from Eq.(2). The outcome of Eq.(2) is implemented into the process. Once the steady state is reached, the outputs of the process are measured to update and solve Eq.(1). The update of gives the ML-NMA the ability to adapt the MA to the changing conditions of .

|  |  |
| --- | --- |
|  | (2) |

**3. Results and discussion**

The ML-NMA was tested in the Otto-Williams reactor. The process consisted of an isothermal CSTR working at a given temperature with two influents ( and ). Inside the CSTR three chemical reactions are produced, while in the approximated model of the process only two of them are considered. The decision variables of the process are and . In this work we have considered as an unmeasured disturbance changing over time. The RTO looks for and those optimize the economic benefit of the process inside a feasible region [4]. The main result of this work was that the evolution of calculated with ML-NMA followed the trajectory of the optimum of the process closer than other MA approaches, while was better estimated by the DUAL-MA SSKF (Figure 2). Nevertheless DUAL-MA SSKF depends on the accuracy in estimation.



**Figure 2.** Evolution of and : ML-NMA (black solid line), real optimum of the process (red dotted line), NMA using Generalized Pattern Search (blue solid line), MA with dual approach and Steady-state Kalman Filter (magenta solid line)

**4. Conclusions**

It has been demonstrated that ML-NMA allows tracking the optimum of an uncertain process which is affected by unmeasured disturbances.

**References**

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