Advanced-multi-step Moving Horizon Estimation

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Abstract: Moving Horizon Estimation (MHE) is an important optimization-based approach for state estimation and parameter updates, because of its capabilities in dealing with nonlinearity and state constraints. In addition, one of the applications is to provide the full state information for Model Predictive Controller (MPC) to control the process in either setpoint tracking or economic control purposes. However, the computational burden of MHE could deteriorate the control performance if the feedback delay caused by computation is too long, leading to potential safety issues or process damage. In this paper, we propose a fast moving horizon estimation algorithm to overcome the long computational time of MHE for real-time control applications, especially for fast dynamics or large-scale systems. We exploit the nonlinear programming (NLP) sensitivity and make use of efficient NLP solvers, IPOPT and k_aug, to reduce the on-line computational costs. This new approach is demonstrated on a CSTR process, where results are compared to ideal MHE and advanced-step MHE (asMHE).

Keywords: Estimation Algorithms, Optimal Estimation, Nonlinear Programming, Sensitivity

1. INTRODUCTION

Moving Horizon Estimation has recently become more popular, especially for model based control strategies such as Nonlinear Model Predictive Control (NMPC). By solving an optimization problem at each sampling time that possesses a sequence of noised measurements, MHE provides the full state information and real-time updates for changing parameters. The former information can be set as the required initial condition of NMPC and the latter updates can improve the performance of NMPC with more accurate parameters. In addition, compared to the well-known Extended Kalman Filter (EKF) (Bryson and Ho (1975), Jazwinski (1970)), the advantages of MHE are its abilities to handle nonlinearities with first principles models and to deal with constraints in a simple and consistent way (Haseltine and Rawlings (2005)). These constraints enable us to include more physical information of the states, leading to better performance of the estimator by avoiding the infeasible region.

However, the non-negligible on-line computing time required for MHE raises some concerns. Reducing computational delay is also important for chemical processes. A delayed state estimate incurs a deadtime in control action, which leads to loss of control performance as well as possible destabilization of the process (Findeisen and Allgöwer (2004), Diehl et al. (2005), Chen et al. (2000)). Some methods to cope with on-line computational load include applying the generalized Gauss-Newton method to a simultaneous framework of the estimation problem in Kraus et al. (2006) and Wynn et al. (2014). In particular, Zavala et al. (2008) proposed a real-time MHE algorithm to tackle the online computational burden with nonlinear programming (NLP) sensitivity. In his approach, the measurements for the next step are predicted by the plant model and the MHE problem is solved offline with the predicted measurements in background. Once the actual measurements are obtained, the optimal solution based on the true measurements is updated quickly using NLP sensitivity. This online updating approach only performs a backsolve for the linear system in each step, and requires less computation time compared to solving a full MHE problem. Nonetheless, this approach can only apply to cases where the MHE solution time is less than one sampling time; this may not be suitable for fast dynamic systems or large-scale plants.

Following on our previous work on advanced-multi step NMPC (amsNMPC, Kim et al. (2020b)), we propose the advanced-multi step MHE (amsMHE) requiring only one processor to handle the longer solution time for MHE. Basically, we predict a number of future measurements with plant model and solve the MHE a few steps ahead depending on how long it takes to obtain the optimal solution in background. When we obtain the actual measurements, we place them in the corresponding position inside the horizon window, update the solution with NPL sensitivity, and retrieve the current estimates. The main difference from asMHE is that we now solve the MHE problem over
multiple sampling times. In addition, the results from this MHE problem would then be used for multiple time steps until the next MHE result is available.

This paper is organized as follows. In section 2, we introduce the formulation of MHE and NLP sensitivity. Section 3 presents the algorithm of amsMHE. Section 4 shows the CSTR case study results and compares them to ideal MHE and asMHE. Finally, section 5 concludes this paper and provides some future perspectives.

2. IDEAL MHE AND NLP SENSITIVITY

Consider the nonlinear system having the state disturbances \( w_k \) and measurement noise \( v_k \):

\[
\begin{align*}
x_{k+1} &= f(x_k, w_k) \\
y_k &= h(x_k) + v_k.
\end{align*}
\]

At time step \( t_k \), we have the past measurement data from the initial time \( t_0 \). Using the whole measurement data makes the size of the estimation problem increase with time. To address this, the MHE formulation with finite horizon \( N \) is introduced with the arrival cost, which approximates the estimation errors from initial time to \( t_k-N \), along with the prior estimate of \( x_{k-N} \) and its covariance. There are several approaches to calculate the arrival costs such as using EKF, unscented KF, or using the information from the NLP solution (Negrete, 2011; Zavala et al., 2007). The last approach is used in this study.

The ideal MHE formulation for estimating the states from the measurement data is as follows:

\[
\begin{align*}
\mathcal{M}_N(\eta_k) : & \\
\min_{z_l, w_l} & \psi_N(\eta_k) = \Gamma(z_{-N}) + \sum_{l=-N}^{-1} L_{N+l}(z_l, w_l) + L_{N}(z_0) \\
\text{s.t.} & \quad z_{l+1} = f(z_l, w_l), l = -N, \ldots, -1 \\
& \quad z_1 \in \mathbb{Z}, w_2 \in \mathbb{W}.
\end{align*}
\]

Here, the arrival cost is:

\[
\Gamma(z_{-N}) = \frac{1}{2}(z_{-N} - \bar{z}_{-N})^\top \Pi_{-N}^{-1}(z_{-N} - \bar{z}_{-N}),
\]

the stage costs are:

\[
L_{N+l} = \frac{1}{2}(y_{k+l} - h(z_l))^\top R_l^{-1}(y_{k+l} - h(z_l))
\]

\[+ \frac{1}{2} w_l^\top Q_l^{-1} w_l, l = -N, \ldots, -1 \]

\[
L_{N} = \frac{1}{2}(y_{k} - h(z_0))^\top R_0^{-1}(y_{k} - h(z_0))
\]

and the prior estimate of \( x_{k-N} \) and its covariance are denoted as \( \bar{z}_{-N} \) and \( \Pi_{-N} \), respectively. \( \eta_k \) is the data set, \( [\bar{z}_{-N}, \Pi_{-N}, y_{k-N}, y_{k-N-1}, \ldots, y_k] \), which fully defines \( \mathcal{M}_N \). When we consider this data set as parameters \( p \), the Karush–Kuhn–Tucker (KKT) conditions can be represented as implicit functions of \( p \):

\[
\phi(s(p)) = 0
\]

where \( s(p) = [z_{-N}^\top, w_{-N}^\top, \lambda_{N+1}^\top, \ldots, z_1^\top, w_1^\top, \lambda_{-1}^\top, z_0^\top] \).

In this study, we investigate the effects of perturbations of \( p \) on the optimal MHE solution. To this end, we adapt the general NLP sensitivity theorem to the MHE problem. Consider \( \eta_k \) in \( \mathcal{M}_N(\eta_k) \) as the nominal parameter \( p_0 \), and assume the following.

Assumption 1. \( f(\cdot), \Gamma(\cdot), \) and \( L(\cdot) \) are twice continuously differentiable in a neighborhood of the nominal solution \( s^*(p_0) \).

Assumption 2. \( s^*(p_0) \) satisfies the linear independence constraint qualifications (LICQ), second order sufficient conditions (SOSC), and strict complementary slackness (SC).

Then, by the NLP sensitivity theorem (Fiacco, 1976, 1983), there exists an isolated, continuous, and differentiable solution vector \( s^*(p) \) for \( p \) in a neighborhood of \( p_0 \). In addition, \( \frac{\partial s}{\partial p} \mid_{p_0} \) is bounded and unique. From this, we can apply the implicit function theorem to (5) and it yields:

\[
K^*(p_0) \frac{\partial s^*(p)}{\partial p} \mid_{p_0} = -\frac{\partial \phi(s(p))}{\partial p} \mid_{p_0}.
\]

where \( K^*(p_0) \) denotes the KKT matrix of \( \mathcal{M}_N(p_0) \). For \( p \) in a neighborhood of \( p_0 \), the first-order Taylor expansion of \( s^*(p) \) is

\[
s^*(p) \approx s^*(p_0) + \frac{\partial s^*(p)}{\partial p} \mid_{p_0} (p - p_0) = \hat{s}(p).
\]

The KKT matrix is nonsingular by Assumption 1 (Nocedal and Wright, 2006) and using (6), we have

\[
\hat{s}(p) = s^*(p_0) - K^*(p_0)^{-1}\frac{\partial \phi(s(p))}{\partial p} \mid_{p_0} (p - p_0)
\]

\[
= s^*(p_0) + \frac{\partial s}{\partial p} \mid_{p_0} (p - p_0).
\]

where, \( \frac{\partial s}{\partial p} = -K^*(p_0)^{-1}\frac{\partial \phi(s(p))}{\partial p} \mid_{p_0} \) is the sensitivity matrix. Thus, we can approximate the optimal solution of \( \mathcal{M}_N(p) \) as \( \hat{s}(p) \), using the optimal solution of \( \mathcal{M}_N(p_0) \) and its sensitivity matrix. Moreover, the errors between the approximate solution and the optimal solution are bounded by

\[
\| \hat{s}(p) - s^*(p) \| \leq L_s \| p - p_0 \|^2
\]

with a constant \( L_s > 0 \). Thus \( s^*(p) - \hat{s}(p) = O(\| p - p_0 \|^2) \).

3. FAST AMS-MHE ALGORITHM

We propose an advanced-multi-step MHE algorithm to avoid the online computational load when more than one sampling time is required to solve MHE problem. The nominal MHE problem with the predicted measurements is solved offline beforehand. The optimal solution of MHE with the real measurements is approximated using NLP sensitivity online. The detailed algorithm is as follows:

**Offline during \( t_k - t_{k+N} \):**

1. Predict the future measurements \( \hat{y}_{k+1}, \ldots, \hat{y}_{k+2N_s-1} \)

\[
x(k+i) = f(x(k+i-1), \hat{w}(k+i-1))
\]

\[
\hat{y}_{k+i+1} = h(\hat{x}_{k+i+1})
\]

\[
i = 1, \ldots, 2N_s - 1
\]

\[
x(k) = \hat{x}(k)
\]

The first \( N_s - 1 \) disturbances can be approximated by the previous MHE problem solved at \( t_{k-N_s} \), while other disturbances are assumed to be zero. That is, \( \hat{w}(k+i-1) = 0, i = N_s, \ldots, 2N_s - 1 \). \( \hat{x}(k) \) denotes the estimated values of states at \( t_k \).
Define the extended data $\tilde{y}_k = (\hat{z}_N(k), \hat{\Pi}_N^{-1}(k), y(k-N), ..., y(k), \hat{y}(k+1), ..., \hat{y}(k+2N_s-1))$ and solve the extended problem $M_{N+2N_s-1}(p_0)$ with $p_0 = \tilde{y}_k$.

$$M_{N+2N_s-1}(p_0) : \begin{align*}
\min_{z_i, w_i} \psi_{N+2N_s-1}(p_0) \\
\text{s.t. } z_{i+1} = f(z_i, w_i), \quad l = -N, ..., 2N_s - 2 \\
z_i \in \mathbb{Z}, \quad w_i \in \mathbb{W}
\end{align*}$$

where,

$$\psi_{N+2N_s-1}(p_0) = \Gamma(z_{-N}) + \sum_{l=-N}^{2N_s-2} L_{N+l}(z_i, w_i)$$

$$\Gamma(z_{-N}) = \frac{1}{2} (z_{-N} - \bar{z}_{N+N_s+1}^k)^\top \hat{\Pi}_N^{-1} (z_{-N} - \bar{z}_{N+N_s+1}^k)$$

$$L_{N+l} = \frac{1}{2} (y_{k+l} - h(z_i))\top R^{-1}_i (y_{k+l} - h(z_i)) + \frac{1}{2} w_i^\top Q^{-1}_l w_i, \quad l = -N, ..., 0$$

(11)

Before $t_{k+N_s}$, obtain the solution $\hat{s}(\tilde{y}_k)$ and then calculate and compute the sensitivity matrix $\frac{\partial \psi}{\partial \tilde{y}_k}$.

**On-line, at** $t_{k+1}$, $i = N_s, ..., 2N_s - 1$:

Note that at this point, the measurements $y(k+j), j = 1, ..., N_s - 1$ are already obtained while $M_{N+2N_s-1}(\tilde{y}_k)$ is solved.

(1) Obtain the measurement $y(k+i)$ and update the current problem data $\eta(k+i) = (\hat{z}_{-N}(k), \hat{\Pi}_N^{-1}(k), y(k-N), ..., y(k+i), \hat{y}(k+i+1), ..., \hat{y}(k+2N_s-1))$.

(2) Using all $N + 1 + i$ measurements in $\eta(k+i)$, compute an instantaneous approximate solution $\hat{s}(\eta(k+i))$ using (8).

(3) Extract the updated solution $\hat{z}_i$ corresponding to the nominal optimal solution $z^*_i$; these are the estimated states, $\hat{x}(k+i) = \hat{z}_i$.

**At** $t_{k+N_s}$:

(1) Set $k$ to $k + N_s$, and prepare the next iteration. We set $\hat{\tilde{y}}(k+i-1) = \hat{w}_i, \quad i = N_s, ..., 2N_s - 1$, which is extracted from the updated solution $\hat{s}(\eta(k))$. $\bar{z}_{-N}(k)$ is set as $\bar{z}_{-N+N_s}$. The arrival cost $\hat{\Pi}_N^{-1}(k)$ is approximated using the inverse of reduced Hessian.

Note that the solution of the MHE problem $M_{N+2N_s-1}(\tilde{y}_k)$ initiated at $t_k$ is used to estimate states only between $t_{k+N_s}$ and $t_{k+2N_s-1}$. The states within $t_k$ and $t_{k+N_s-1}$ are estimated using the previous MHE solution, initiated at $t_{k-N_s}$.

## 4. SIMULATION RESULTS

The proposed amsMHE is applied to a CSTR, where the exothermic reaction $A \rightarrow B$ occurs. The dimensionless dynamic models in Hicks and Ray (1971); Yang and Biegler (2013) are used with the state disturbances $w_1$ and $w_2$.

$$\begin{align*}
\frac{dx_1}{dt} &= \frac{1}{w_2} (1 - x_1) - k' \exp(-E' / x_2)^3 + w_1 \\
\frac{dx_2}{dt} &= \frac{1}{w_2} (x_f - x_2) + k' \exp(-E' / x_2)^3 + w_2 \\
y &= x_2
\end{align*}$$

$x_1$ and $x_2$ are the dimensionless A concentration and temperature, respectively. $x_f$ is measured. $x_f$ and $x_e$ are the dimensionless feed concentration and temperature, respectively. $k'$ and $E'$ are the dimensionless rate constant and ratio of the activation energy to the gas constant, respectively. $A_h$ is the dimensionless heat transfer area. The first manipulated variable $u_1$ is the reactor jacket heat transfer coefficient which increases monotonically as the coolant flow rate increases. The second manipulated variable $u_2$ is $V/F$ where $F$ is the feed flow rate and $V$ is the reactor volume. In addition, model parameters are $x_f = 0.395, x_e = 0.382, k' = 17328, E' = 5$ and $A_h = 1.95 \times 10^{-4}$. The moving horizon length $N_s$ is set as 20 steps with the sampling time of 1 s. The constraints for the states are $[0, 1]$ because both are dimensionless values.

The continuous model is discretized by Lagrange-Radau collocation method, and it is solved using Pyomo (Hart et al., 2011) and IPOPT 3.12 (Wächter and Biegler, 2006) with the linear solver MA57 (Duff, 2004). The KKT matrix and the inverse of the reduced Hessian are obtained using $k_{aug}$ (Thierry and Biegler, 2019).

### 4.1 With state disturbances and measurement noise

We simulate four different cases with the state disturbance $w$ and measurement noise $v$:

- Case 1: $w_{x_1}$ and $w_{x_2} \sim N(0, 0.01^2)$, $v \sim N(0, 0.01^2)$
- Case 2: $w_{x_1}$ and $w_{x_2} \sim N(0, 0.02^2)$, $v \sim N(0, 0.01^2)$
- Case 3: $w_{x_1}$ and $w_{x_2} \sim N(0, 0.01^2)$, $v \sim N(0, 0.02^2)$
- Case 4: $w_{x_1}$ and $w_{x_2} \sim N(0, 0.02^2)$, $v \sim N(0, 0.02^2)$

We use the fixed control inputs obtained by the ideal NMPC and the ideal MHE for the amsMHE ($N_s = 1$) and amsMHE ($N_s = 3$) simulation. The $R_l$ and $Q_l$ are set as the standard deviation of each noise.

The results are shown in Fig. 1 and Table 1. The sum-of-squared errors for amsMHE are smaller than for ideal MHE. Although the sum-of-squared errors in $x_2$ for cases 3 and 4 are smaller for amsMHE, the total sum-of-squared errors are always greater than those of ideal MHE.

To investigate why amsMHE can yield better estimations than ideal MHE, we analyze the KKT conditions of ideal MHE and the approximate update of amsMHE. This occurs because the MHE objective function contains the
state disturbance terms. In section 4.2, we show the results of the case without state disturbances, where the objective function does not include them and the ideal MHE estimates the true values better than asMHE.

Consider the KKT conditions of the ideal MHE at \( t_{k+1} \) where the data set \( \eta_{k+1} = \{z_{N}, z_{N-1}, y_{k}, y_{k-1}, \ldots, y_{2}, y_{1}\} \) is used with \( N \) horizon, and the inequality constraints are assumed inactive. The Lagrangian of \( M_N(\eta_{k+1}) \) is

\[
L = \psi_N(\eta_{k+1}) + \sum_{l=N+1}^{0} \lambda_{l+1}^T (z_{l+1} - f(z_l, w_l)).
\]

and the KKT conditions for \( z_1 \) and \( \lambda_1 \) are,

\[
\nabla_{z_1} L = -\nabla_{z_1} h_1^T R_1^{-1}(y_{k+1} - h(z_1)) + \lambda_1 = 0 \quad (15a)
\]

\[
\nabla_{\lambda_1} L = z_1 - f(z_0, w_0) = 0 \quad (15b)
\]

\[
\nabla_{w_0} L = Q_0^{-1} w_0 - \nabla_{w_0} f_{0}^T \lambda_1 = 0. \quad (15c)
\]

Here, \( h_1 = h(z_1) \) and \( f_1 = f(z_1, w_1) \). The solution of ideal MHE \( z_1^*, w_0^* \), and \( \lambda_1^* \) satisfies (15). In addition, because \( h(z_1) = [0, 1] \), for this example, (18a) is simplified as

\[
\lambda_1^* = \left[ \begin{array}{c} \lambda_1^* \\ R_1^{-1}(y_{k+1} - x_{2}^* t_{k+1}) \end{array} \right]
\]

With \( \eta_0 = \{z_{N}, z_{N-1}, y_{k}, y_{k-1}, \ldots, y_{2}, y_{1}\} \) and an extended horizon \( N+1 \), the Lagrangian of asMHE becomes:

\[
L_{as} = \psi_N(\eta_{k+1}) + \sum_{l=N}^{0} \lambda_{l+1}^T (z_{l+1} - f(z_l, w_l)).
\]

The solution \( z_{1, as}, w_{0, as}, \) and \( \lambda_{1, as} \) of \( M_N(\eta_{k+1}) \) satisfies the following parts of the KKT conditions:

\[
\nabla_{z_1} L_{as} = -\nabla_{z_1} h_1^T R_1^{-1}(y_{k+1} - h(z_1)) + \lambda_1 = 0 \quad (18a)
\]

\[
\nabla_{\lambda_1} L_{as} = z_1 - f(z_0, w_0) = 0 \quad (18b)
\]

\[
\nabla_{w_0} L_{as} = Q_0^{-1} w_0 - \nabla_{w_0} f_{0}^T \lambda_1 = 0. \quad (18c)
\]

When the measurement \( y_{k+1} \) is obtained, the solution is updated to satisfy

\[
\nabla_{z_1} L_{as} \Delta z_1 + \Delta \lambda_1 - \nabla_{z_1} h_1^T R_1^{-1} \Delta p = 0 \quad (19)
\]

where the variables \( \Delta z_1 = z_1 - z_{1, as}, \Delta \lambda = \lambda_1 - \lambda_{1, as}, \) and \( \Delta p = y_{k+1} - y_{k+1} \). Because \( h(z_1) = [0, 1] \), for this example, (18a) becomes

\[
\left[ \begin{array}{c} 0 \\ R_1^{-1}(y_{k+1} - x_{2, as}^* t_{k+1}) \end{array} \right] + \lambda_{1, as} = 0
\]

and (19) becomes

\[
0 + \lambda_{1, as} = 0
\]

From (20) and (21),

\[
\left[ \begin{array}{c} 0 \\ R_1^{-1}(\bar{x}_2 t_{k+1}^* - x_{2, as}^* t_{k+1}) \end{array} \right] + \lambda_1 - \left[ \begin{array}{c} 0 \\ R_1^{-1} y_{k+1} \end{array} \right] = 0.
\]

and

\[
\lambda_1 = \left[ \begin{array}{c} 0 \\ R_1^{-1}(y_{k+1} - \bar{x}_2 t_{k+1}) \end{array} \right].
\]

Considering (15c) and (18c) and comparing (16) and (23), we can note that the estimates of \( x_2 t_{k+1}^* \) depend on the estimates of state disturbances \( w_0 \) in addition to \( z_0 \). This may make the asMHE estimate of \( x_2 t_{k+1} \) better from the perspective of the errors.

On the other hand, as seen in Table 1 for asMHE with \( N_s = 3 \), solving the optimization problem less frequently, and with less accurate predicted measurements, leads to a deterioration of estimation performance. In addition, the asMHE approximates an ideal MHE with real and predicted measurements depending on the time steps. This can also affect estimation performance.

Table 1. The squared errors between the estimates and true values of asMHE with \( N_s = 3 \), asMHE, and ideal MHE when considering state disturbances and measurement noise.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \sum_{t=0}^{50} (x_1 - \hat{x}_1)^2 )</th>
<th>( \sum_{t=0}^{50} (x_2 - \hat{x}_2)^2 )</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0473</td>
<td>0.0081</td>
<td>0.1054</td>
</tr>
<tr>
<td>2</td>
<td>0.0601</td>
<td>0.0113</td>
<td>0.0714</td>
</tr>
<tr>
<td>3</td>
<td>0.1074</td>
<td>0.0194</td>
<td>0.2068</td>
</tr>
<tr>
<td>4</td>
<td>0.3953</td>
<td>0.044</td>
<td>0.1572</td>
</tr>
</tbody>
</table>

5. CONCLUSION

This paper proposes an advanced-multi-step MHE that the optimization problem with predicted outputs is solved in advance, and the optimal estimates with the real measurements are approximated by NLP sensitivity update online.
Fig. 1. State estimation with state disturbances and measurement noise.

Table 3. Average and maximum CPU times for solving ideal MHE and amsMHEs.

<table>
<thead>
<tr>
<th></th>
<th>amsMHE</th>
<th>asMHE</th>
<th>Ideal MHE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Offline</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CPU time [s]</td>
<td>Average</td>
<td>0.0042</td>
<td>0.0070</td>
</tr>
<tr>
<td></td>
<td>Max</td>
<td>0.0316</td>
<td>0.0456</td>
</tr>
<tr>
<td>Online</td>
<td>Average</td>
<td>0.0005</td>
<td>0.0000</td>
</tr>
<tr>
<td>CPU time [s]</td>
<td>Max</td>
<td>0.0156</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

We investigate the performances of amsMHE, asMHE and ideal MHE with state disturbances and measurement noise. The estimation performance of asMHE is sometimes better than ideal MHE because general MHE problems minimize the sum of estimation errors and the norm of state disturbances. On the other hand, given the stochastic nature of these simulations, it is expected that performance comparisons among these approaches may be case dependent. Also, when we simulate the cases only with measurement noise, we observe that the performance deteriorates as $N_s$ increases. The computational load of NLP can be handled by ams strategy, solving the optimization problem in background; thus, future work will consider large-scale problems to show the computational advantages of the amsMHE method. Also, parametric uncertainties will be considered, and the amsMHE method will be coupled with advanced-multi-step nonlinear model predictive control (amsNMPC), thus leading to a fast output-based controller.

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Fig. 2. State estimation without state disturbances and only with measurement noise.

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