Problem formulation and efficient numerical methods of real-time estimation based on DAE process models

Ihno Schrot

Outline: 1. Introduction | 2. Problem formulation 2.1 Moving Horizon approach | 3. Numerical solution 3.1 Multiple Shooting as framework for MHE 3.2 Solution of the NLP 3.3 real-time iteration | 4. Discussion

Output and state noise MHE

$$
\begin{aligned}
\min_{\boldsymbol{x}_j,\ \boldsymbol{z}_j,\ \boldsymbol{p},\ \boldsymbol{w}_j} \quad & \left(\left\| \begin{matrix} \boldsymbol{x}_L - \bar{\boldsymbol{x}}_L \\ \boldsymbol{p}_L - \bar{\boldsymbol{p}}_L \end{matrix} \right\|_{P_L}^2 + \sum_{j=L}^{k} ||\boldsymbol{y}_j - \boldsymbol{h}(\boldsymbol{x}(\tau_j) \quad, \boldsymbol{z}(\tau_j), \boldsymbol{p})||_{V_j}^2 + \sum_{j=L}^{k-1} ||\boldsymbol{w}_j||_W^2 \right) \\
\text{s.t.} \quad & \boldsymbol{x}_{j+1} = \boldsymbol{F}(\boldsymbol{x}_j, \boldsymbol{z}_j, \boldsymbol{u}_j, \boldsymbol{p}) + \boldsymbol{w}_j, \qquad j = L, \dots, k-1, \\
& \boldsymbol{0} = \boldsymbol{g}(\boldsymbol{x}_j, \boldsymbol{z}_j, \boldsymbol{u}_j, \boldsymbol{p}), \qquad j = L, \dots, k, \\
& \boldsymbol{x}_{j,\min} \le \boldsymbol{x}_j \le \boldsymbol{x}_{j,\max}, \qquad j = L, \dots, k, \\
& \boldsymbol{z}_{j,\min} \le \boldsymbol{z}_j \le \boldsymbol{z}_{j,\max}, \qquad j = L, \dots, k, \\
& \boldsymbol{w}_{j,\min} \le \boldsymbol{w}_j \le \boldsymbol{w}_{j,\max}, \qquad j = L, \dots, k, \\
& \boldsymbol{p}_{\min} \le \boldsymbol{p} \le \boldsymbol{p}_{\max}.
\end{aligned} \tag{MHE}
$$

Optimal arrival cost

$$
\begin{aligned}
C_{L+1}^* = \min_{\boldsymbol{x}_L,\ \boldsymbol{p}_L} \quad & \left(\left\| \begin{matrix} \boldsymbol{x}_L - \bar{\boldsymbol{x}}_L \\ \boldsymbol{p}_L - \bar{\boldsymbol{p}}_L \end{matrix} \right\|_{P_L}^2 + ||\boldsymbol{y}_L - \boldsymbol{h}(\boldsymbol{x}(\tau_L), \boldsymbol{p}_L)||_{V_L}^2 + \left\| \begin{matrix} \boldsymbol{w}_L \\ \boldsymbol{w}_L^p \end{matrix} \right\|_{\bar{W}_L}^2 \right) \\
\text{s.t.} \quad & \boldsymbol{w}_L = \boldsymbol{x}_{L+1} - \boldsymbol{F}(\boldsymbol{x}_L, \boldsymbol{u}_L, \boldsymbol{p}_L), \\
& \boldsymbol{w}_L^p = \boldsymbol{p}_{L+1} - \boldsymbol{p}_L.
\end{aligned} \tag{ACP}
$$

QR decomposition

$$
M_{\mathrm{QR}} = \left(\begin{array}{c|c} P_L & 0 \\ -(V_L H_X \mid V_L H_p) & 0 \\ -\bar{W}_L \begin{pmatrix} X_X & X_p \\ 0 & \mathbb{I} \end{pmatrix} & \bar{W}_L \end{array} \right) = Q \begin{pmatrix} \mathcal{R}_1 & \mathcal{R}_{12} \\ 0 & \mathcal{R}_2 \\ 0 & 0 \end{pmatrix} \tag{1}
$$

$$
\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} := Q^T \begin{pmatrix} -P_L \begin{pmatrix} \bar{\boldsymbol{x}}_L \\ \bar{\boldsymbol{p}}_L \end{pmatrix} \\ V_L(\boldsymbol{y}_L - \tilde{\boldsymbol{h}}) \\ \bar{W}_L \begin{pmatrix} \tilde{\boldsymbol{x}} \\ 0 \end{pmatrix} \end{pmatrix}. \tag{2}
$$

$$
P_{L+1} := \mathcal{R}_2, \quad \begin{pmatrix} \bar{\boldsymbol{x}}_{L+1} \\ \bar{\boldsymbol{p}}_{L+1} \end{pmatrix} = -\mathcal{R}_2^{-1} \rho_2. \tag{3}
$$

Quadratic subproblem

$$
\begin{aligned}
\min_{\Delta \boldsymbol{r}_k^i} \quad & \left\| J(\boldsymbol{r}_k^i; \boldsymbol{D}_k) + \nabla_{\boldsymbol{r}} J(\boldsymbol{r}_k^i; \boldsymbol{D}_k)^T \Delta \boldsymbol{r}_k^i \right\|_2^2 \\
\text{s.t.} \quad & \boldsymbol{0} = \boldsymbol{G}(\boldsymbol{r}_k^i; \boldsymbol{D}_k) + \nabla_{\boldsymbol{r}} \boldsymbol{G}(\boldsymbol{r}_k^i; \boldsymbol{D}_k)^T \Delta \boldsymbol{r}_k^i, \\
& \boldsymbol{0} \le \boldsymbol{H}(\boldsymbol{r}_k; \boldsymbol{D}_k) + \nabla_{\boldsymbol{r}} \boldsymbol{H}(\boldsymbol{r}_k; \boldsymbol{D}_k)^T \Delta \boldsymbol{r}_k^i
\end{aligned} \tag{QP}
$$

Algorithm 1: MHE real-time iteration

Input: multiple shooting data vector:

$\boldsymbol{r}_{k-1} = (\boldsymbol{x}_{L-1}, \boldsymbol{z}_{L-1}, \dots, \boldsymbol{x}_{k-1}, \boldsymbol{z}_{k-1}, \boldsymbol{w}_{L-1}, \dots, \boldsymbol{w}_{k-2}, \boldsymbol{p})$

online data set from previous intervals:

$\boldsymbol{D}_{k-1} = (\bar{\boldsymbol{x}}_{L-1}, \bar{\boldsymbol{p}}_{L-1}, P_{L-1}, \boldsymbol{y}_{L-1}, V_{L-1}, \boldsymbol{u}_{L-1}, \dots, \boldsymbol{y}_{k-1}, V_{k-1}, \boldsymbol{u}_{k-1},)$

online data which becomes known during the iteration:

$\boldsymbol{y}_k$, V_k, $\boldsymbol{u}_k$

Output: current estimates $\hat{\boldsymbol{x}}_k,\ \hat{\boldsymbol{z}}_k,\ \hat{\boldsymbol{p}}_k,$

updated $\boldsymbol{r}_k$ and updated $\bar{\boldsymbol{x}}_L,\ \bar{\boldsymbol{p}}_k$ for $\boldsymbol{D}_k$

At initial sample $k = 0$ provide initial guess $\boldsymbol{w}_0,\ \boldsymbol{D}_0$

for *samples* $k = 1, 2, \dots$ **do**

  Preparation phase *for horizon* $[\tau_L, \tau_k]$ ***before*** τ_k **:**

    Update arrival cost data $(\bar{\boldsymbol{x}}_L, \bar{\boldsymbol{p}}_L)$ and P_L with eq. (3)

    Shift data vectors:

      $\boldsymbol{r}_k^- = (\boldsymbol{x}_L, \boldsymbol{z}_L, \dots, \boldsymbol{x}_k^-, \boldsymbol{z}_k^-, \boldsymbol{w}_L, \dots, \boldsymbol{w}_{k-1}^-, \boldsymbol{p})$

      $\boldsymbol{D}_k = (\bar{\boldsymbol{x}}_L, \bar{\boldsymbol{p}}_L, P_L, \boldsymbol{y}_L, V_L, \boldsymbol{u}_L, \dots, *, V_k, \boldsymbol{u}_k)$

      where $*$ is a wildcard for the not yet known output $\boldsymbol{y}_k$

    Solve DAE system on interval $[\tau_{k-1}, \tau_k]$ and set

      $\boldsymbol{x}_k^- := \boldsymbol{x}(\tau_k; \boldsymbol{x}_{k-1}, \boldsymbol{z}_{k-1})$

      $\boldsymbol{w}_{k-1}^- = 0$

      $\boldsymbol{z}_k^- := \boldsymbol{z}(\tau_k; \boldsymbol{x}_{k-1}, \boldsymbol{z}_{k-1})$

    Compute *all but one vector* component of problem [QP]

      except for $V_k(\boldsymbol{y}_k - \boldsymbol{h}(\boldsymbol{x}_k, \boldsymbol{z}_k, \boldsymbol{p}))$

    Compute *all matrix* components of problem [QP]

  end of preparation phase

  Estimation phase *for horizon* $[\tau_{L+1}, \tau_k]$ ***at*** τ_k **:**

    Complete vector $\boldsymbol{D}_k$ as $\boldsymbol{y}_k$ becomes known

    Solve [QP] for $\Delta \boldsymbol{r}_k$

    Update:

      $\boldsymbol{r}_k = \boldsymbol{r}_k^- + \Delta \boldsymbol{r}_k$

      $\hat{\boldsymbol{x}}_k = \boldsymbol{x}_k$

      $\hat{\boldsymbol{z}}_k = \boldsymbol{z}_k$

      $\hat{\boldsymbol{p}}_k = \boldsymbol{p}$

  end of estimation phase

end

List of Symbols

Symbol	Description	Element of/size
C_L	Arrival cost of time window $[\tau_L, \tau_k]$; the superscripts "$*$" and "$'$" denote variants	$\mathbb{R}$
$\boldsymbol{D}_k$	Online data in the MHE at time τ_k	No actual mathematical dimension
$\Delta \boldsymbol{r}_k^i$	i-th increment for $\boldsymbol{r}_k$ in the Gauß-Newton method for the MHE	see $\boldsymbol{r}_k$
$\boldsymbol{F}$	Iteration function for $\boldsymbol{x}_j$ usually obtained from numerical integration	$\mathbb{R}^{n_x} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$
$\boldsymbol{f}$	Function in the DAE system	$\mathbb{R}^{n_x} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$
$\boldsymbol{G}$	Collected equality constraints in terms of $\boldsymbol{r}_k$ and $\boldsymbol{D}_k$ in the MHE	$(M-1)n_x + Mn_z$ equations
$\boldsymbol{g}$	Function in the DAE system	$\mathbb{R}^{n_x} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_z}$
$\boldsymbol{H}$	Collected inequality constraints in terms of $\boldsymbol{r}_k$ and $\boldsymbol{D}_k$ in the MHE	$2M(2n_x + n_z) + 2n_p$ inequalities
$\boldsymbol{h}$	Ideal measurement function (collecting all devices in one vector)	$\mathbb{R}^{n_x} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_h}$
H_p	Sensitivity matrix of the ideal measurement function with states at time τ_{L+1} with respect to the parameters $\boldsymbol{p}$	$\mathbb{R}^{n_h \times n_p}$
H_x	Sensitivity matrix of the ideal measurement function with states at time τ_{L+1} with respect to the initial values $\boldsymbol{x}(\tau_L)$	$\mathbb{R}^{n_h \times n_x}$
J	General cost function for the optimal control problem	$\mathbb{R}^{n_x} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}$
k	Index of last measurement in time window of MHE	$\mathbb{R}$
L	$:= k-M+1$; Index of first measurement in time window of MHE	$\mathbb{R}$
M	Number of measurements in time window of MHE	$\mathbb{R}$
M_{QR}	Matrix which is decomposed with a QR-decomposition. See equation (1)	$\mathbb{R}^{(2n_x+2n_p+n_h)\times(2n_x+2n_p)}$
$\boldsymbol{p}$	System parameters	$\mathbb{R}^{n_p}$
P_L	Weighting matrix for the arrival cost C_L	$\mathbb{R}^{(n_x+n_p)\times(n_x+n_p)}$
$\bar{\boldsymbol{p}}_L$	Parameter for the arrival cost C_L	$\mathbb{R}^{n_p}$
$\hat{\boldsymbol{p}}$	Estimation of the parameters	$\mathbb{R}^{n_p}$
Q	Orthogonal matrix of QR-decomposition of M_{QR}	$\mathbb{R}^{(2n_x+2n_p+n_h)\times(2n_x+2n_p+n_h)}$
$\boldsymbol{q}$	Optimization variables for the discretised controls in the multiple shooting method	$\mathbb{R}^{n_u}$
$\mathcal{R}_1,\ \mathcal{R}_{12},\ \mathcal{R}_2$	Matrices occuring in the QR-decomposition of M_{QR} (see equation (1))	$\mathbb{R}^{(n_x+n_p)\times(n_x+n_p)}$
$\rho_1,\ \rho_2,\ \rho_3$	Needed in the computation of the arrival cost; see equation (2) for definition	$\mathbb{R}^{(n_x+n_p)}$ for $\rho_1,\ \rho_2$, $\mathbb{R}^{n_h}$ for ρ_3
$\boldsymbol{r}_k$	Collected optimization variables in the MHE at time τ_k	$\mathbb{R}^{(M)*(n_x+n_z)+(M-1)*n_x+n_p}$
$\boldsymbol{r}_k^i$	i-th iterate for $\boldsymbol{r}_k$ in the Gauß-Newton method for the MHE	see $\boldsymbol{r}_k$
$\boldsymbol{s}^x,\ \boldsymbol{s}^z$	Initial states at the shooting nodes in the multiple shooting method	$\mathbb{R}^{n_x},\ \mathbb{R}^{n_z}$
T	End time (in the offline case)	$\mathbb{R}$
t	Time	$\mathbb{R}$

Symbol	Description	Element of/size
t_0	Starting time (in the offline case)	$\mathbb{R}$
t_{M}	Length of time window of MHE	$\mathbb{R}$
τ_j	j-th sampling time/shooting node of the multiple shooting method	$\mathbb{R}$
$\boldsymbol{u}$	Controls	$\mathbb{R}^{n_u}$
V	Weighting matrix of the measurement noise. Usually square root of the inverse of the covariance matrix of $\boldsymbol{v}$	$\mathbb{R}^{n_h \times n_h}$
$\boldsymbol{v}$	Measurement noise	$\mathbb{R}^{n_h}$
$\boldsymbol{w}$	State noise	$\mathbb{R}^{n_x}$
$\boldsymbol{w}^p$	Parameter noise	$\mathbb{R}^{n_p}$
W	Weighting matrix of the state noise. Usually square root of the inverse of the covariance matrix of the state noise $\boldsymbol{w}$	$\mathbb{R}^{n_x \times n_x}$
$\bar{W}$	Weighting matrix of the combined state and parameter noise. Usually square root of the inverse of the combined covariance matrix of $\boldsymbol{w}$ and $\boldsymbol{w}^p$	$\mathbb{R}^{(n_x+n_p)\times(n_x+n_p)}$
$\boldsymbol{x}$	Differential states	$\mathbb{R}^{n_x}$
$\boldsymbol{x}_0$	Initial values for differential states	$\mathbb{R}^{n_x}$
X_p	Sensitivity matrix of the states at time τ_{L+1} with respect to the parameters $\boldsymbol{p}$	$\mathbb{R}^{n_x \times n_p}$
X_x	Sensitivity matrix of the states at time τ_{L+1} with respect to the initial values $\boldsymbol{x}(\tau_L)$	$\mathbb{R}^{n_x \times n_x}$
$\bar{\boldsymbol{x}}_L$	Parameter for the arrival cost C_L	$\mathbb{R}^{n_x}$
$\hat{\boldsymbol{x}}$	Estimation of the differential states	$\mathbb{R}^{n_x}$
$\boldsymbol{\xi}$	Collected optimization variables in the multiple shooting method	bla
$\boldsymbol{y}_j$	Output of measurement devices	$\mathbb{R}^{n_h}$
$\boldsymbol{z}$	Algebraic states	$\mathbb{R}^{n_z}$
$\hat{\boldsymbol{z}}$	Estimation of the algebraic states	$\mathbb{R}^{n_z}$

Note: A subscript either indicates the interval index for which the variable holds or that the variables was taken at time τ_j unless specified otherwise.

References

Hans Georg Bock. Numerical treatment of inverse problems in chemical reaction kinetics. In *Modelling of chemical reaction systems*, pages 102–125. Springer, 1981.

Hans Georg Bock. *Randwertproblemmethoden zur Parameteridentifizierung in Systemen nichtlinearer Differentialgleichungen*. Number 183. Der Math.-Naturwiss. Fakultät der Universität Bonn, 1987.

Hans Georg Bock and Karl-Josef Plitt. A multiple shooting algorithm for direct solution of optimal control problems. *IFAC Proceedings Volumes*, 17(2):1603–1608, 1984.

Fred Daum. Nonlinear filters: beyond the kalman filter. *IEEE Aerospace and Electronic Systems Magazine*, 20(8):57–69, 2005.

Arthur Gelb. *Applied optimal estimation*. MIT press, 1974.

Peter Kühl, Moritz Diehl, Tom Kraus, Johannes P. Schlöder, and Hans Georg Bock. A real-time algorithm for moving horizon state and parameter estimation. *Computers & Chemical Engineering*, 35(1):71 – 83, 2011.

James B. Rawlings and Bhavik R. Bakshi. Particle filtering and moving horizon estimation. *Computers & Chemical Engineering*, 30(10):1529 – 1541, 2006.

Stephen Wright and Jorge Nocedal. Numerical optimization. *Springer Science*, 35(67-68):7, 1999.