Dynamic identification of boundary conditions for convection-diffusion transport model subject to noisy measurements

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Abstract. The paper addresses the problem of dynamic identification of boundary conditions for one-dimensional convection-diffusion transport model based on noisy measurements of the function of interest. Using finite difference method the original model with the partial differential equation is replaced with the discrete linear dynamic system model with noisy multisensor measurements in which boundary conditions are included as the unknown input vector. To solve the problem, the algorithm of simultaneous the state and input vector estimation is used. The results of numerical experiments are presented which confirm the practical applicability of the proposed approach.

1. Introduction and problem statement

In recent decades there has been an increased interest in inverse problems for partial differential equations in various areas of science and technology. There is a great demand to develop new methods for solving applied problems that require processing and interpretation of experimental data [1]. Among the various types of inverse problems, boundary inverse problems are of great importance. In these problems, the behavior of the unknown function on the boundary of the considered region is investigated.

The important class of models widely used to describe natural and man-made processes and phenomena are convection-diffusion transport models [2, 3].

In the simplest one-dimensional case, the convection-diffusion transport model can be described by equation (1) with initial condition (2) and boundary conditions (3):

\[
\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2}, \quad a < x < b, 0 < t < +\infty, \tag{1}
\]

\[
c(x, 0) = \varphi(x), \quad a \leq x \leq b, \tag{2}
\]

\[
c(a, t) = f_1(t), c(b, t) = f_2(t), \quad 0 < t < +\infty, \tag{3}
\]

where \(c(x, t)\) is the function of interest, \(x\) is the spatial variable, \(t\) is the time variable, \(v\) is the convection rate, \(\alpha\) is the diffusion coefficient, \(\varphi(x)\), \(f_1(t)\), \(f_2(t)\) are given functions, \(a\), \(b\) are the bounds of the considered segment.
Consider the problem of dynamically (in real time) estimating the values of the function \( c(x,t) \) in the model (1)–(3) at the ends of the segment \([a, b]\) based on noisy measurements of its values at the internal points of the segment at successive discrete time moments. Such tasks arise in practice when the behavior of an object or process on the boundary of the considered region is not directly measurable or involves high costs. In contrast to the classical formulations, we are interested not in the analytical expressions for the functions \( f_1(t) \) and \( f_2(t) \), but in the estimates of their numerical values at discrete time moments.

2. Discrete linear dynamic system model

To solve the problem let us move from the original model (1)–(3) to the discrete linear dynamic system in state space with noisy measurements which in general case has the following form:

\[
\begin{align*}
  c_k &= F_{k-1}c_{k-1} + B_{k-1}u_{k-1} + w_{k-1}, \\
  z_k &= H_k c_k + \xi_k, \\
  k &= 1, 2, \ldots,
\end{align*}
\]

where \( c_k \in \mathbb{R}^n \) is the system state vector, \( u_k \in \mathbb{R}^r \) is the input vector, \( z_k \in \mathbb{R}^m \) is the measurements vector, noises \( w_k \in \mathbb{R}^q \) and \( \xi_k \in \mathbb{R}^m \) are independent normally distributed sequences with zero mean and covariance matrices \( Q \geq 0 \) and \( R > 0 \), correspondingly.

Let us consider in the plane \( Oxt \) a regular grid with spatial step \( \Delta x \), time step \( \Delta t \), and points \((x_i, t_k)\):

\[ x_i = a + i\Delta x, \quad t_k = k\Delta t, \quad i = 0, 1, \ldots, N, \quad k = 0, 1, \ldots \]

Denote \( c_i^k = c(x_i, t_k), \varphi_i = \varphi(x_i), f_1^k = f_1(t_k), f_2^k = f_2(t_k) \) and write down the finite-difference scheme for (1)–(3):

\[
\begin{align*}
  \frac{c_i^{k+1} - c_i^k}{\Delta t} + \frac{c_{i+1}^{k+1} - 2c_i^{k+1} + c_{i-1}^{k+1}}{2\Delta x} &= \alpha \frac{c_{i-1}^k - 2c_i^k + c_{i+1}^k}{\Delta x^2}, \quad i = 1, 2, \ldots, N - 1, \quad k = 1, 2, \ldots, \ (4) \\
  c_i^0 &= \varphi_i, \quad i = 0, 1, \ldots, N, \ (5) \\
  c_i^k &= f_1^k, \quad c_i^N = f_2^k, \quad k = 1, 2, \ldots \ (6)
\end{align*}
\]

From equation (4) it follows that the value of \( c(x,t) \) in \( k \)-th time row is determined by its values in \((k - 1)\)-th time row:

\[
   c_i^k = (r_1 + r_2)c_{i-1}^{k-1} + (1 - 2r_2)c_i^{k-1} + (r_2 - r_1)c_{i+1}^{k-1}, \ (7)
\]

where \( r_1 = \frac{\Delta t}{2\Delta x}, \quad r_2 = \frac{\alpha \Delta t}{\Delta x^2} \). Let us rewrite (7) as

\[
   c_i^k = a_1 c_{i-1}^{k-1} + a_2 c_i^{k-1} + a_3 c_{i+1}^{k-1},
\]

where \( a_1 = r_1 + r_2, \quad a_2 = 1 - 2r_2, \quad a_3 = r_2 - r_1 \).
Now the discrete linear stochastic system model can be represented as follows:

\[
\begin{bmatrix}
  c_1^1 \\
  c_2^1 \\
  \vdots \\
  c_{k-1}^1 \\
  \cdots \\
  c_{k-2}^n \\
  c_k^n
\end{bmatrix}
= 
\begin{bmatrix}
  a_2 & a_3 & 0 & \cdots & 0 & 0 & 0 \\
  a_1 & a_2 & a_3 & \cdots & 0 & 0 & 0 \\
  0 & a_1 & a_2 & a_3 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
  0 & 0 & 0 & \cdots & a_2 & a_3 & 0 \\
  0 & 0 & 0 & \cdots & a_1 & a_2 & a_3 \\
  0 & 0 & 0 & \cdots & 0 & a_1 & a_2 \\
  \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{bmatrix}
\begin{bmatrix}
  c_1^{k-1} \\
  c_2^{k-1} \\
  \vdots \\
  c_{k-1}^{k-1} \\
  \cdots \\
  c_{k-2}^{n-2} \\
  c_k^n
\end{bmatrix}
+ 
\begin{bmatrix}
  a_1 & 0 \\
  0 & 0 \\
  0 & 0 \\
  \vdots & \vdots \\
  0 & 0 \\
  0 & 0 \\
  0 & a_3
\end{bmatrix}
\begin{bmatrix}
  f_1^{k-1} \\
  f_2^{k-1} \\
  \vdots \\
  f_{k-1}^{k-1} \\
  \vdots \\
  f_{k-2}^{n-2} \\
  u_{k-1}
\end{bmatrix}
\]

(8)

where \( n = N - 1 \) (the state vector \( c_k \) consists of all internal points of the spatial grid), \( H_k \in \mathbb{R}^{m \times n} \) is the observation matrix, \( m \) is the number of measured components of the state vector.

Model (8) is a deterministic discrete linear dynamic system with noisy measurements in which unknown boundary conditions are included in the two-dimensional input vector \((r = 2)\).

System matrix \( F_k \in \mathbb{R}^{n \times n} \) is a three-diagonal constant matrix, input matrix \( B_k \in \mathbb{R}^{n \times 2} \) is also constant.

Different methods of optimal estimation theory may be used to identify unknown parameters of the constructed model. For example in [4], for identification of coefficients \( v \) and \( \alpha \) in (1) authors use the approach based on the combination of least squares method and extended Kalman filter. But the input vector was assumed known.

3. Algorithm for simultaneous estimation of the state vector and unknown input

We suppose that the input vector \( u \) of the model (8) is unknown. Earliest approaches to its estimation were based on augmenting the state with an unknown input, where a prescribed model for the unknown input is assumed.

In this paper for dynamic identification of boundary conditions, we suggest using the algorithm for simultaneous estimation of the state vector and the unknown input developed in [5]. This work is an extension of [6] and [7] but it proposes a recursive filter with a joint estimation of the unknown input and the state vector.

Suppose that the condition

\[
\text{rank} \, H_k B_{k-1} = \text{rank} \, B_{k-1} = r
\]

holds for each \( k \).

Denote by \( I_n, I_m, I_p \) identity matrices of order \( n, m \) and \( p \) correspondingly \((p = m - r)\).

**Algorithm 1.** (S. Gillijns, B. De Moor [5]).

**for** \( k = 1, 2, \ldots \) **do**

**begin**

1) predict \( c_k \) and \( P_k \) without using the input estimate

\[
\hat{c}_{k|k-1} = F_{k-1} \hat{c}_{k-1|k-1},
\]

\[
P_{k|k-1} = F_{k-1} P_{k-1|k-1} F_{k-1}^T + Q_{k-1},
\]

**end**

**for** \( k = 2, 3, \ldots \) **do**

**begin**

2) update \( c_k \) and \( P_k \) using the input estimate

\[
\hat{c}_{k|k} = \hat{c}_{k|k-1} + H_k (z_k - H_k \hat{c}_{k|k-1} - \hat{c}_{k|k-1}),
\]

\[
P_{k|k} = (I_k - K_k H_k) P_{k|k-1},
\]

where \( K_k = P_{k|k-1} H_k^T (H_k P_{k|k-1} H_k^T + R_k)^{-1} \)

**end**
2) estimate the input vector
\[ \tilde{R}_k = H_k P_{k|k-1} H_k^T + R_k, \]
\[ D_k = H_k B_{k-1}, \]
\[ M_k = (D_k^T \tilde{R}_k^{-1} D_k)^{-1} D_k^T \tilde{R}_k^{-1}, \]
\[ \dot{u}_{k-1} = M_k(z_k - H_k \hat{c}_{k|k-1}), \] (10)

3) predict \( c_k \) and \( P_k \) using the input estimate
\[ \hat{c}_{k|k} = \hat{c}_{k|k-1} + B_{k-1} \dot{u}_{k-1}, \]
\[ P_{k|k} = (I_n - B_{k-1} M_k H_k) P_{k|k-1} (I_n - B_{k-1} M_k H_k)^T + B_{k-1} M_k R_k M_k^T B_{k-1}^T, \]

4) update \( c_k \) and \( P_k \)
\[ \tilde{R}_k^* = (I_m - H_k B_{k-1} M_k) \tilde{R}_k (I_m - H_k B_{k-1} M_k)^T, \]
\[ S_k^* = -B_{k-1} M_k R_k, \]
\[ \alpha_k = [0 \ I_p] U_k^T \tilde{S}_k^{-1}, \]
\[ K_k = (P_{k|k}^* H_k^T + S_k^*) \alpha_k^T (\alpha_k \tilde{R}_k^* \alpha_k^T)^{-1} \alpha_k, \]
\[ \hat{c}_{k|k} = \hat{c}_{k|k} + K_k(z_k - H_k \hat{c}_{k|k}), \] (12)
\[ P_{k|k} = P_{k|k}^* - K_k (P_{k|k}^* H_k^T + S_k^*)^T. \]

end

In (11) matrix \( \tilde{S}_k \) is such that \( \tilde{S}_k \tilde{S}_k^T = \tilde{R}_k \), and \( U_k \) is orthogonal matrix of left singular eigenvectors of matrix \( \tilde{S}_k^{-1} H_k B_{k-1} \).

4. Numerical Experiments
Consider the following problem:
\[ \frac{\partial c}{\partial t} + 2 \frac{\partial c}{\partial x} = \frac{\partial^2 c}{\partial x^2}, \quad 0 < x < 1, 0 < t < +\infty, \] (13)
\[ c(x, 0) = 0, \quad 0 \leq x \leq 1, \] (14)
\[ c(0, t) = f_1(t), c(1, t) = f_2(t), \quad 0 < t < +\infty, \] (15)

where \( c(x, t) \) is the concentration of the pollutant in the one-dimensional flow moving from left to right,
\[ f_1(t) = 4 |3t - [3t + 0.5]|, \quad f_2(t) = \begin{cases} 0, & t \leq 0.5, \\ 2t - 1, & t < 0.5. \end{cases} \]

The condition (14) means that the initial pollutant concentration on the considered segment equals to 0. The first boundary condition (15) corresponds to a periodic increase of the pollutant concentration at the left bound according to the law of a triangle wave with period 1/3. The second boundary condition may be considered as an absorption wall up to time 0.5, followed by a linear increase of the pollutant concentration at the right bound.

Consider the spatial grid with step \( \Delta x = 0.2 \), consisting of four internal points \( x_1 = 0.2, x_2 = 0.4, x_3 = 0.6, x_4 = 0.8 \) and two boundary points \( x_0 = 0, x_5 = 1 \). Time step \( \Delta t \) is
taken equal to $\Delta x^2 = 0.01$ according to the convergence condition. Numerical experiments were conducted in Matlab.

Figure 1 shows the plot of the solution of \((13)-(15)\) obtained by the finite-difference method for $t \in [0; 1]$ ($k = 1, 2, \ldots, 100$).

Consider the measurement model with two sensors ($m = 2$) located at the first and last internal points of the grid. Note, that for such model condition \((9)\) is satisfied. System \((8)\) for this case is as follows:

$$
\begin{bmatrix}
    c_1^k \\
    c_2^k \\
    c_3^k \\
    c_4^k
\end{bmatrix}
= 
\begin{bmatrix}
    0.5 & 0.2 & 0 & 0 \\
    0.3 & 0.5 & 0.2 & 0 \\
    0 & 0.3 & 0.5 & 0.2 \\
    0 & 0 & 0.3 & 0.5
\end{bmatrix}
\begin{bmatrix}
    c_1^{k-1} \\
    c_2^{k-1} \\
    c_3^{k-1} \\
    c_4^{k-1}
\end{bmatrix}
+ 
\begin{bmatrix}
    0.3 & 0 \\
    0 & 0 \\
    0 & 0 \\
    0 & 0.2
\end{bmatrix}
\begin{bmatrix}
    f_1^{k-1} = c_5^{k-1} \\
    f_2^{k-1} = c_6^{k-1}
\end{bmatrix},$$

$$
\begin{bmatrix}
    z_1^k \\
    z_2^k
\end{bmatrix}
= 
\begin{bmatrix}
    1 & 0 & 0 & 0 \\
    0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
    c_1^k \\
    c_2^k \\
    c_3^k \\
    c_4^k
\end{bmatrix}
+ 
\begin{bmatrix}
    \xi_1^k \\
    \xi_2^k
\end{bmatrix},
$$

\(k = 1, 2, \ldots\) 

Figure 2 shows the plots of noisy measurements in the first and last internal points. Figures 3 and 4 show the results of estimating the boundary values of the function $c(x,t)$. Figure 5 shows the plot of the solution estimate (in internal points and on the boundary) obtained by algorithm 1 with noise covariance $R = \text{diag}\{0.03^2, 0.03^2\}$. Note, that for the considered model at each iteration of the algorithm we use formula \((10)\) to calculate the estimate of the input vector for the previous discrete time moment and we use formula \((12)\) to obtain the estimate of the state vector for the current discrete time moment.

Thus, the evaluation of the boundary values of the function $c(x,t)$ (input vector in the model) is made with a delay of one time moment, and at the last iteration of the algorithm, it is not
Figure 2. Noisy measurements \( (x = 0.2 \text{ and } x = 0.8) \).

Figure 3. Left bound \( (x = 0) \).

Table 1 shows the mean square errors (RMSE) of the function \( c(x, t) \) in the boundary and internal points of the grid and the normalized mean square error (nRMSE) with different noise estimated.
Figure 4. Right bound ($x = 1$).

Figure 5. Estimation of the solution.
Table 1. Estimation errors.

|       | RMSE_{left} | RMSE_1 | RMSE_2 | RMSE_3 | RMSE_4 | RMSE_{right} | nRMSE |
|-------|-------------|--------|--------|--------|--------|---------------|-------|
| R_1   | 1.1085      | 0.2983 | 0.1047 | 0.0797 | 0.3062 | 1.6743        | 2.0572|
| R_2   | 0.0986      | 0.0289 | 0.0135 | 0.0103 | 0.0311 | 0.1639        | 0.1967|
| R_3   | 0.0118      | 0.0032 | 0.0011 | 0.0009 | 0.0030 | 0.0172        | 0.0214|

5. Conclusion
The paper proposes a new approach to the dynamic identification of boundary conditions in the model of convection-diffusion transport with noisy measurements, based on the use of discrete filtering methods.

The novelty of the proposed approach lies in the transition from the original model described by the partial differential equation to a discrete linear dynamic system in which the boundary conditions are represented as unknown input effects, for the identification of which the algorithm of S. Gillijns and B. De Moor is used.

Further research will be aimed at the development of the proposed approach and new methods for solving inverse problems for the model of convection-diffusion transport from experimental data.

6. References
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