Optimal Input Design for Model Discrimination
Based on Kullback Divergence

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Abstract: The optimal input design problem has been discussed for efficient order determination of autoregressive models under the input power constraint. By solving a mathematical programming problem, auto-caovariance sequence of an optimal input is derived, which maximizes the time-average of the Kullback divergence to make difference of the models bigger without making much effect on the original system behavior. The proposed approach is based on the sequential comparison of the AIC, and it can be applied to find the model structure of general linear time-invariant discrete-time systems.

1. INTRODUCTION

System identification deals with constructing mathematical models of dynamical systems from observed input/output data. In order to obtain the maximal information from the observation data, the idea of optimal experimental design originally developed for static regression analysis (Fedorov [1972], Silvey [1980], Pukelsheim [1993]) has been extensively applied (Mehra [1974], Goodwin and Payne [1977], Zarrop [1979], Forsell and Ljung [2000], Hildebrand and Gevers [2003]). Most studies on this aspect were for optimal input design for accurate parameter estimation within a specified model structure under some constraints on input or output, assuming the precise knowledge of the underlying model structure of the data generating processes. However, in many cases such knowledge is not available and hence the analysis of the data should be performed in two steps: identification of an appropriate model structure from a given class of competing models; and parameter estimation in the specified model structure. Despite the universal recognition of the importance of the first step in system identification, the studies on the optimal input design for this step is quite few, see Kabaila (Goodwin and Payne [1977]), Uosaki et al. [1984] and Uosaki et al. [1987]. These considerations are related to the hypothesis testing approach (Atkinson and Cox [1974], Dette [1995]) and the information criterion approach (Akaike [1974]). See also Uosaki and Hatanaka [2005].

Here, the optimal input design problem for structure determination of autoregressive model is considered. An optimal input is derived, which enlarges the distance of the two rival models, and does not deviate from the original model without input, where the distance of models are measured by the Kullback divergence.

2. PROBLEM STATEMENT

Consider the following stable autoregressive (AR) model,

\[
y(t) = \sum_{k=1}^{p} a_k y(t-k) + \varepsilon(t)
\]  

(1)

where \( \varepsilon(t) \) is independently normally distributed with mean zero and variance \( \sigma^2 \). Model structure determination problem here is to determine the order of the AR model (1). An useful criterion for selection of such nesting models is Akaike’s Information Criterion (AIC) (Akaike [1974]), which is an estimate of the Kullback discrimination information measure (KDI) (Kullback [1994]) and offers a relative measure of the information loss when a given model is used to describe reality. The criterion may be minimized over choices of \( p \) to form a tradeoff between the fit of the model measured by the sum of squared residuals, and the model’s complexity measured by \( p \), and the model minimizing the criterion is chosen as the suitable model. Thus the following two AR models based on the observation sequence \( y^T = (y(t), y(t-1), \ldots, y(1))^T \) can be compared.

\[
M_1 : y(t) = \sum_{k=1}^{n} a_k^{(1)} y(t-k) + \varepsilon^{(1)}(t)
\]

(2)

\[
M_2 : y(t) = \sum_{k=1}^{n-1} a_k^{(2)} y(t-k) + \varepsilon^{(2)}(t)
\]

with independently normally distributed random variables \( \varepsilon^{(j)}(t) \) with mean zero and variance \( \sigma^{(j)2} \) (\( j = 1, 2 \)).

It is assumed that a controllable input \( u(t-1) \) can be added to the model in order to determine the order efficiently and the problem how to design a suitable input \( u(t-1) \) will be considered. By introducing the input \( \{u(t-1)\} \), the models corresponding to the AR models with order \( n \) and \( n-1 \) changes to the autoregressive models with exogenous input (ARX models),
\[ M'_1: y(t) = \sum_{k=1}^{n} a^{(1)}_k y(t-k) + u(t-1) + \varepsilon^{(1)}(t) \]
\[ M'_2: y(t) = \sum_{k=1}^{n} a^{(2)}_k y(t-k) + u(t-1) + \varepsilon^{(2)}(t) \]
or
\[ M'_1: A_1(z^{-1})y(t) = u(t-1) + \varepsilon^{(1)}(t) \]
\[ M'_2: A_2(z^{-1})y(t) = u(t-1) + \varepsilon^{(2)}(t) \]

with
\[ A_1(z^{-1}) = 1 - \sum_{k=1}^{n} a^{(1)}_k z^{-k} \]
\[ A_2(z^{-1}) = 1 - \sum_{k=1}^{n} a^{(2)}_k z^{-k} \]

where \( z^{-1} \) is a delay operator. Model discrimination can be accelerated by enlarging the distance between the two models (3). However, the system behaviors such as the output process \( \{y(t)\} \) may change due to the added input \( \{u(t)\} \). The large deviations of the behaviors from the original model (1) are not suitable, and hence, the input should be chosen not to affect the model so much. This implies that the distance between the original AR models \( M_k \) and the ARX models \( M'_k (k = 1, 2) \) should be small as possible. Further, the following input power constraint
\[ E[u^2(t)] \leq C \]
with a given constant \( C \) is imposed from a practical point of view.

Thus the optimal input design for model discrimination can be summarized as follows:

(P0) "Find a input \( \{u(t)\} \) such that it maximizes the distance between models \( M'_1 \) (autoregressive model of order \( n \) with a controllable input) and \( M'_2 \) (autoregressive model of order \( n-1 \) with a controllable input) under the restrictions on the distance between models \( M_k \) (autoregressive model) and \( M'_k \) (autoregressive model with a controllable input) \( (j = 1, 2) \) and the input power constraint (6)."

Since the AIC closely relates to the Kullback discrimination information measure (KDI), the following Kullback divergence \( J_t[M_k : M'_t; y^t, u^{t-1}] \) is employed as a measure of distance between the models \( M_k \) and \( M'_t \)
\[ J_t[M_k : M'_t; y^t, u^{t-1}] = I_t[M_k : M'_t; y^t, u^{t-1}] + I_t[M'_t : M_k; y^t, u^{t-1}] \]

where \( I_t[M_k : M'_t; y^t, u^{t-1}] \) is the Kullback discrimination information measure,
\[ I_t[M_k : M'_t; y^t, u^{t-1}] = \int_{-\infty}^{\infty} p_t(y|u^{t-1}) \log \frac{p_t(y|u^{t-1})}{p_t(y|u^{t-1})} dy \]

where \( p_t(y|u^{t-1}) \) is the probability density function of \( y \) given \( u^{t-1} = (u(t-1), \ldots, u(1)) \) under the model \( M_t \) \( (t = 1, 2) \).

It is known that the Kullback divergence has the following properties:

[Properties]
(i) The Kullback divergence is non-negative,
\[ J_t[M_k : M'_t; y^t, u^{t-1}] \geq 0 \]
(ii) The Kullback divergence equals to zero if and only if the models are identical, i.e., \( p_k(y^t|u^{t-1}) = p_t(y^t|u^{t-1}) \).
(iii) The Kullback divergence is symmetric,
\[ J_t[M_k : M'_t; y^t, u^{t-1}] = J_t[M'_t : M_k; y^t, u^{t-1}] \]

These facts suggest that it becomes easier to discriminate the models as the divergence \( J_t[M'_1 : M'_2; y^t, u^{t-1}] \) is larger since the distance between the models is larger. Therefore, it is natural to find an input which maximizes \( J_t[M'_1 : M'_2; y^t, u^{t-1}] \). The following theorem shows that the Kullback divergence can be decomposed shown as in Hatanaka and Uosaki [1995].

[Theorem]
The Kullback divergence can be decomposed as
\[ J_t[M'_1 : M'_2; y^t, u^{t-1}] = J_t^{(0)}[M'_1 : M'_2; y^t, u^{t-1}] + J_t^{(1)}[M'_1 : M'_2; y^t, u^{t-1}] + J_t^{(2)}[M'_1 : M'_2; y^t, u^{t-1}] + J_t^{(3)}[M'_1 : M'_2; y^t, u^{t-1}] \]

where
\[ J_t^{(1)}[M'_1 : M'_2; y^t, u^{t-1}] = \frac{1}{2\sigma^{(1)}_2} \int_{-\infty}^{\infty} \left( \frac{A_2(z^{-1})}{A_1(z^{-1})} - 1 \right)^2 u(t-1)^2 \]
\[ J_t^{(2)}[M'_1 : M'_2; y^t, u^{t-1}] = \frac{1}{2\sigma^{(2)}_2} \int_{-\infty}^{\infty} \left( \frac{A_2(z^{-1})}{A_1(z^{-1})} - 1 \right)^2 u(t-1)^2 \]
\[ J_t^{(3)}[M'_1 : M'_2; y^t, u^{t-1}] = \frac{1}{2\sigma^{(3)}_2} \int_{-\infty}^{\infty} \left( \frac{A_2(z^{-1})}{A_1(z^{-1})} - 1 \right)^2 \frac{dz}{z} \]

Here, \( J_t^{(1)}[M'_1 : M'_2; y^t, u^{t-1}] \) indicates the difference in noise components, and \( J_t^{(2)}[M'_1 : M'_2; y^t, u^{t-1}] \) and \( J_t^{(3)}[M'_1 : M'_2; y^t, u^{t-1}] \) indicate the differences in input and output relations between two models, respectively.

Since they are all non-negative and equals to zero if and only if the models are identical as \( J_t[M'_1 : M'_2; y^t, u^{t-1}] \), only the input-dependent term \( J_t^{(2)}[M'_1 : M'_2; y^t, u^{t-1}] \), or its time average
\[ \bar{J}_t^{(2)}[M'_1 : M'_2; y, u] = \lim_{t \to \infty} \frac{1}{t} \int_{0}^{t} J_t^{(2)}[M'_1 : M'_2; y^t, u^{t-1}] \]

can be considered for efficient model discrimination. Thus the problem can be restated as

(P1) "Find a input \( \{u(t)\} \) such that it maximizes the time-average of the input-dependent term of the Kullback divergence, \( \bar{J}_t^{(2)}[M_1 : M_2; y, u] \) under the constraints
\[ \bar{J}_t^{(2)}[M_1 : M_2; y, u] \leq L \]
\[ \bar{J}_t^{(2)}[M_2 : M_2; y, u] \leq L \]
with a given constant \( L \), and input power constraint given by (6).”

3. OPTIMAL INPUT DESIGN

An optimal input is derived, which maximizes \( J(2)[M'_1: M'_2; y, u] \) defined by (11) under the constraints (12). Suppose that the input sequence \( \{u(t)\} \) is a zero-mean stationary ergodic Gaussian process. Then, the output sequence \( \{y(t)\} \) is also a zero-mean stationary ergodic Gaussian process by the stable linear system assumption. By the ergodic property assumption, the time average in (11) can be replaced by the ensemble average,

\[
J(2)[M'_1: M'_2; y, u] = \lim_{t \to \infty} \frac{1}{t} J(2)[M'_1: M'_2; y', u'-1]
\]

\[
= E[J(2)[M'_1: M'_2; y', u'-1]]
\]

\[
= E \left[ \frac{1}{2\sigma(2)^2} \left( \frac{A_2(z^{-1})}{A_1(z^{-1})} - 1 \right) u(t-1)^2 \right]
\]

\[
+ E \left[ \frac{1}{2\sigma(1)^2} \left( \frac{A_1(z^{-1})}{A_2(z^{-1})} - 1 \right) u(t-1)^2 \right]
\]

Define

\[
\hat{u}(t) = \frac{1}{(\sigma(1)^2)A_1(z^{-1})A_2(z^{-1})} u(t)
\]

Then the ensemble average of \( J(2)[M'_1: M'_2; y', u'-1] \) can be expressed by

\[
J(2)[M'_1: M'_2; y, u] = \frac{1}{2} \left[ E[(\sigma(1)^2)(A_2(z^{-1}) - A_1(z^{-1}))A_2(z^{-1})\hat{u}(t-1)^2] \right]
\]

\[
+ E[(\sigma(2)^2)(A_1(z^{-1}) - A_2(z^{-1}))A_1(z^{-1})\hat{u}(t-1)^2]
\]

Let

\[
H_1(z^{-1}) = \sigma(1)(A_2(z^{-1}) - A_1(z^{-1}))A_2(z^{-1})
\]

\[
= \sum_{k=1}^{2n-1} h_k^{(1)} z^{-k}
\]

\[
H_2(z^{-1}) = \sigma(2)(A_1(z^{-1}) - A_2(z^{-1}))A_1(z^{-1})
\]

\[
= \sum_{k=1}^{2n} h_k^{(2)} z^{-k}
\]

where

\[
h_k^{(1)} = \sigma(1)(a_1^{(1)} - a_1^{(2)})
\]

\[
h_k^{(1)} = \sigma(1)(a_1^{(2)} - a_2^{(2)}) - \sum_{l=1}^{k-1} a_1^{(2)}(a_1^{(1)} - a_1^{(2)})
\]

\[
k = 2, \ldots, n - 1
\]

\[
= \sigma(1) \sum_{l=1}^{k-n} a_1^{(2)}(a_1^{(1)} - a_1^{(2)})
\]

\[
k = n + 1, \ldots, 2n - 1
\]

\[
h_k^{(2)} = \sigma(2)(e_1^{(1)} - e_1^{(2)})
\]

\[
h_k^{(2)} = \sigma(2)(a_1^{(2)} - a_2^{(2)}) - \sum_{l=1}^{k-1} a_1^{(2)}(a_1^{(1)} - a_1^{(2)})
\]

\[
k = 2, \ldots, n - 1
\]

\[
h_k^{(2)} = \sigma(2) \sum_{l=1}^{k-n} a_1^{(2)}(a_1^{(1)} - a_1^{(2)})
\]

\[
k = n + 1, \ldots, 2n - 1
\]

Thus,

\[
J(2)[M'_1: M'_2; y, u] = \frac{1}{2} \left[ E \left[ \sum_{k=1}^{2n} h_k^{(1)} \hat{u}(t-1) \right]^2 \right]
\]

\[
+ E \left[ \sum_{k=1}^{2n} h_k^{(2)} \hat{u}(t-1) \right]^2
\]

and this can be evaluated by using the following autocovariance of the filtered input \( \hat{u}(t) \),

\[
\rho_k = E[\hat{u}(t)\hat{u}(t-k)] \quad (k = 0, 1, \ldots, 2n - 1)
\]

That is,

\[
J(2)[M'_1: M'_2; y, u] = \sum_{k=0}^{2n-1} \alpha_k \rho_k
\]

\[
\alpha_0 = \frac{1}{2} \left( \sum_{k=1}^{2n-1} h_k^{(1)} \right)^2 + \sum_{k=1}^{2n} h_k^{(2)}
\]

\[
\alpha_k = \sum_{l=1}^{2n-k-1} h_l^{(1)} h_{k+l}^{(1)} + \sum_{l=1}^{2n-k} h_l^{(2)} h_{k+l}^{(2)} \quad (k = 1, 2, \ldots, 2n - 2)
\]

\[
\alpha_{2n-1} = h_1^{(2)} h_{2n}^{(2)}
\]

Since the input \( u(t) \) is expressed by using the filtered input \( \hat{u}(t) \) as

\[
u(t) = \sigma(1)^2 A_1(z^{-1}) A_2(z^{-1}) \hat{u}(t)
\]

\[
= \sigma(1)^2 \sum_{k=0}^{2n-1} a_k \hat{u}(t-k)
\]

with

\[
a_0 = 1
\]

\[
\alpha_k = -a_1^{(1)} - a_1^{(2)} - \sum_{l=1}^{n} a_l^{(1)} a_{k-l}^{(2)} \quad (k = 1, \ldots, n - 1)
\]

\[
av_n = -a_1^{(1)} + \sum_{l=1}^{n} a_l^{(1)} a_{n-l}^{(2)}
\]

\[
av_k = \sum_{l=1}^{n} a_l^{(1)} a_{k-l}^{(2)} \quad (k = n + 1, \ldots, 2n - 1)
\]

the input power constraint (6) can be expressed by
\[
0 < E[u^2(t)] = E \left[ \left( \sigma(1) \sigma(2) \sum_{k=0}^{2n-1} \tilde{a}_k \tilde{u}(t - k) \right)^2 \right] = \sigma(1)^2 \sigma(2)^2 \sum_{k=0}^{2n-1} \sum_{k=0}^{2n-1} \beta_k \rho_k \leq C
\]

where \( \rho_k = \rho_0 + \sum_{k=1}^{2n-1} \beta_k \rho_k \), and the conditions (12) can be rewritten as

\[
j^2[\{M_1 : M_1'; y, u\}] = E \left[ \frac{1}{2\sigma(1)^2} - A_1(z^{-1})^{-1} u(t) \right]^2 \leq \frac{1}{2\sigma(1)^2} E[u^2(t-1)] \leq L
\]

and

\[
j^2[\{M_2 : M_2'; y, u\}] = \frac{1}{2\sigma(2)^2} E[u^2(t-1)] \leq L
\]

with \( E[u^2(t-1)] \) that equals to \( E[u^2(t)] \) given by (23). Furthermore, the following conditions are required by the nature of auto-covariances \( \{\tilde{\rho}_k\} \).

\[
\tilde{\rho}_0 > 0 \quad \tilde{R}_{2n-1} \text{ is nonnegative definite}
\]

where \( \tilde{R}_{2n-1} = \begin{bmatrix} \tilde{\rho}_0 & \tilde{\rho}_1 & \ldots & \tilde{\rho}_{2n-1} \\ \tilde{\rho}_1 & \tilde{\rho}_0 & \ldots & \tilde{\rho}_{2n-2} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\rho}_{2n-1} & \tilde{\rho}_{2n-2} & \ldots & \tilde{\rho}_0 \end{bmatrix} \).

Summarizing the above, the optimal input design problem for discriminating two autoregressive models (1) can be reduced to the following mathematical programming problem.

\[
\begin{align*}
\text{(P1)} & \quad \text{Maximize} & 2n-1 \sum_{k=0}^{2n-1} & \alpha_k \tilde{\rho}_k \\
& \quad \text{subject to} & 0 < \beta_0 \tilde{\rho}_0 + 2 \sum_{k=1}^{2n-1} \beta_k \tilde{\rho}_k & \leq C' \\
& & C' & = \min \left( \frac{C}{\sigma(1)^2 \sigma(2)^2}, \frac{2L}{\sigma(1)^2 \sigma(2)^2} \right) \\
& & \tilde{R}_{2n-1} \text{ is nonnegative definite}
\end{align*}
\]

\( \text{(Remark)} \)

For the case of autoregressive model of order 1, this mathematical programming can be reduced to a linear programming problem, as in Section 4, since the positive definiteness of \( \tilde{R}_1 \) leads to the linear constraint. Once the auto-covariances \( \{\tilde{\rho}_k\}, k = 0, 1, \ldots, 2n-1 \), which the optimal filtered input \( \tilde{u}''(t) \) should possesses, can be obtained, the optimal filtered input \( \tilde{u}''(t) \) with this auto-covariances can be realized, for example, by the following Chebyshev system approach (Zarrop [1979], Ng and Qureshi [1981]). The optimal input \( \tilde{u}''(t) \) is chosen as

\[
\tilde{u}''(t) = \sum_{p=1}^{2n-1} m_p \cos(\omega_p t)
\]

where \( r = n/2 \), \( (n + 1)/2 \), \( \omega_i \in [0, 2\pi] \), \( \omega_p \neq \omega_q \), and \( m_j > 0 \). The amplitudes \( \{m_p\} \) and frequencies \( \{\omega_p\} \) satisfy the following system of equations.

\[
\begin{bmatrix}
1 & 1 & \ldots & 1 \\
1 & \cos(\omega_1) & \cdots & \cos(\omega_r) \\
\vdots & \vdots & \ddots & \vdots \\
1 & \cos((n-1)\omega_1) & \cdots & \cos((n-1)\omega_r)
\end{bmatrix}
\begin{bmatrix}
\gamma_1 \\
\gamma_2 \\
\vdots \\
\gamma_r
\end{bmatrix}
= \begin{bmatrix}
\tilde{\rho}_0 - C_0 \\
\tilde{\rho}_1 - C_1 \\
\vdots \\
\tilde{\rho}_{n-1} - C_{n-1}
\end{bmatrix}
\]

and

\[
\gamma_p = \tilde{m}_p^2 \\
f(\omega_p) = A(e^{j\omega_p})A(e^{-j\omega_p}) p = 1, \ldots, r \\
C_k = \frac{\sigma(1)^2}{2} \int_{-\pi}^{\pi} \frac{A(e^{j\omega})A(e^{-j\omega})}{\sigma(2)^2} d\omega k = 0, \ldots, n \\
A(z) = 1 - a_1^{(1)} z^{-1} - a_2^{(1)} z^{-2} - \cdots - a_n^{(1)} z^{-n}
\]

Then the optimal input \( u''(t) \) is easily obtained by

\[
u''(t) = (\sigma(1)^2 + \sigma(2)^2) \sum_{k=0}^{2n-1} \tilde{a}_k \tilde{u}''(t - k)
\]

In practice, the optimal input derived here cannot be employed since the true parameter values are not known before identification experiments, and then the sequential approach can be applied (Gerencsér, et al. [2007]). In the approach, the autoregressive parameters are estimated based on the observation data of input and output, and their estimates are used in the optimal input.

4. NUMERICAL EXAMPLE

Consider the problem to determine the order of the following autoregressive model of order 1,

\[
y(t) = a_1 y(t-1) + \varepsilon(t)
\]

based on its observation sequence \( \{y(t)\} \) by introducing the controllable input \( \{u(t)\} \) with power constraint

\[
E[u^2(t)] \leq C
\]

where \( \varepsilon(t) \) is independently normally distributed with zero mean and variance \( \sigma^2 \).

In this case, an optimal input will be found such that it discriminates the following two rival models.

\[
M_1 : y(t) = a_1^{(1)} y(t-1) + \varepsilon^{(1)}(t) \\
M_2 : y(t) = \varepsilon^{(2)}(t)
\]

The following linear programming problem should be solved. Maximize

\[
\tilde{J}^* = a_1^2 (\sigma(1)^2 + \sigma(2)^2 (1 + a_1^{(1)2})) \tilde{\rho}_0 - 2a_1^{(1)3} \sigma(2)^2 \tilde{\rho}_1
\]
Fig. 1. Object function and feasible region

subject to

\[ \bar{\rho}_0 > 0 \]
\[ \bar{R}_1 = \begin{bmatrix} \bar{\rho}_0 & \bar{\rho}_1 \\ \bar{\rho}_1 & \bar{\rho}_0 \end{bmatrix} \text{is non-negative definite} \]
\[ 0 < (1 + a_1^{(1)} \bar{\rho}_0 - 2 \bar{\rho}_1^2 \bar{\rho}_1) \]
\[ \leq C' = \min \left( \frac{C'}{\sigma_1^{(2)} \sigma_2^{(2)}} \right) \]

The solution is

\[ \bar{\rho}_0 = \frac{C'}{(1 - a_1^2)} - \epsilon \]
\[ \bar{\rho}_1 = \frac{C'}{(1 - a_1^2)} - \frac{(1 + a_1^2)}{4a_1} \epsilon \]
\[ J^* = \frac{a_1^2 a_1^{(12)}}{1 + a_1^2} (2C' - (1 - a_1^2) \epsilon) \]

with very small \( \epsilon > 0 \) to satisfy the inequality condition.

For \( a_1^{(1)} = 0.5 \), \( C' = 1 \), \( L = 0.2 \), dashed lines in Fig 1 are corresponding to the restrictions and the feasible region is the enclosed area by head lines. The objective function shown by solid line in Fig. 1 gives the optimal auto-covariances as \( \{\bar{\rho}_0, \bar{\rho}_1\} \) and the maximum \( J^* = \frac{12}{3} - \frac{1}{3} \).

The optimal input sequence \( \{a^*(t)\} \), and then \( \{\bar{\rho}^*(t)\} \) with these auto-covariances can be constructed by the Chebyshev system approach.

5. CONCLUSIONS

The optimal input design problem has been discussed for efficient order determination of autoregressive models under the input power constraint. By solving a mathematical programming problem, auto-covariance sequence of the optimal input is derived, which maximizes the time-average of the Kullback divergence and makes difference of two rival models bigger without making much effect on the original system behavior. The proposed approach is based on the sequential comparison of the AIC, and it can be applied to find the structure of general linear time-invariant discrete-time systems. Since it sometimes takes much time to reach the final decision, optimal input design for accelerated determination of model structure might be pursued such as multi-model discrimination (Nikoukhah et al. [2002]).

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