

Validity of the standard cross-correlation test for model structure validation^{*}

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Abstract

In the standard prediction error framework of system identification, statistical properties of estimated models are typically derived under the assumption that the true system is in the model class. The standard model structure validation test for plant models is the sample cross-correlation test between the residuals of the model and the input. It turns out that the standard test itself is valid only under exactly those assumptions it is meant to verify, i.e. system is in the model class. It is shown that for reliable results of the validation test a vector-valued test is required and that accurate noise modelling is indispensable for reliable model structure validation. This shows the limitation of separate validation of plant and noise model structures. Improvements of the test are presented, while it is motivated that reserving data only to be used for model validation is not efficient.

Key words: model validation, system identification, undermodelling, model uncertainty, statistical tests

1 Introduction

In system identification, one of the central issues is in quantifying a measure of quality on identified models. In a standard prediction error identification procedure an uncertainty region is constructed around the (nominal) model estimate on the basis of the measurement data and prior assumptions on the data generating process. Particularly in the context of identification for robust control the uncertainty region could be argued to be of more importance than the nominal model. The set of models induced by the uncertainty region has to be guaranteed (at a certain level of probability) to contain the “true system”, i.e. the actual process under consideration, to allow for a robust controller design.

In the system identification theory of the prediction error framework the uncertainty region follows from a parameter covariance matrix associated with a Gaussian distribution corresponding to a stochastic noise assumption [16,23]. This uncertainty region reflects the effect of noise in the measure-

ments on the estimated parameters. The uncertainty region can be said to contain the actual process (at a certain level of probability) if the model errors are due to the noise in the data only and are not due to a limitation of the model structure. Moreover, the available analytical expressions for the (noise-induced) parameter covariance matrix themselves are valid under the assumption that there are no undermodelling errors. That is, the model uncertainty region is correct under the assumption that the true system is in the model class ($S \in \mathcal{M}$).

Since the 1990's a number of model uncertainty bounding techniques have become available which explicitly take the effect of undermodelling into account, see e.g. [9,10,3,13] for approaches that originate from classical statistical approaches, and [22,19,11] for approaches based on model validation in a deterministic worst-case setting. In these approaches bounds on unmodelled dynamics, due to the fact that the chosen model structure is not rich enough to capture the true system, are taken into account in the quantified model uncertainty. The resulting uncertainty bounds can then be used subsequently in a worst-case scenario for purpose of robust controller analysis and synthesis, both in terms of stability and performance.

However instead of explicitly quantifying unmodelled dynamics in identified models, an alternative approach has advocated the use of validated models only, see e.g. [15]. In other words: once a model passes a validation test there is

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no evidence of unmodelled dynamics in the data; the effect of undermodelling can then be neglected since it is indistinguishable from the effects of measurement noise. A practical identification procedure then contains a model structure validation test. The model structure is sequentially enlarged until the resulting model estimate passes the validation test. A best-case scenario is then assumed (“if there is no proof of undermodelling we assume that it is not there”) and a model uncertainty region is constructed based on the noise induced errors only, i.e. it is presumed that $\mathcal{S} \in \mathcal{M}$.

Some critical issues can be raised with respect to this best-case scenario. Even if the effect of undermodelling is indistinguishable from the effects of noise, it may not be negligible. For example, in [18] a bound is derived for an aggregated undermodelling error in models which pass a validation test. Additionally, data-based model validation will always remain dependent on the excitation properties of the input signal used during identification. Nevertheless, the best-case scenario is widely used, and it is obvious that there is a clear need for well-motivated tools that detect whether for given measurement data the appropriate model structure has been chosen.

In this paper a critical evaluation will be performed of the standard model validation test that is current practice in validating an identified plant model \hat{G} . In practice, the cross-correlation test as implemented in the System Identification toolbox of Matlab [17] on the sample cross-correlation between the residuals of the model and the input is used extensively and nearly exclusively. It will appear that although the test works well in many situations, it actually is valid only under exactly the assumption it intends to verify, namely that the system is in the model class.

An improved version of the test is proposed following an asymptotic analysis that is slightly different from the classical situation, implying that less severe (asymptotic) convergence conditions are required for its validity. It is shown that reliable model structure validation of plant models essentially requires accurate noise modelling as well as a vector-valued rather than a pointwise test. The former result puts severe limitations on the possibilities of separately validating of plant and noise models. Simulation examples are included to illustrate the results. The current paper is a revised and extended version of [5].

2 Notation and Problem Setting

We will consider prediction error models parametrized by a parameter vector θ , corresponding to a plant model $G(q, \theta)$ and a noise model $H(q, \theta)$, with q the standard shift operator. In a standard prediction error framework [16,23] a model is identified from measurement data $Z^N := \{y, u\}_N$ of data length N according to

$$\hat{\theta}_N = \arg \min_{\theta} V_N(\theta, Z^N) = \arg \min_{\theta} \frac{1}{N} \sum_{t=1}^N \varepsilon^2(t, \theta), \quad (1)$$

where the so-called residuals $\varepsilon(t, \theta)$ are constructed as

$$\varepsilon(t, \theta) = H^{-1}(q, \theta) (y(t) - G(q, \theta) u(t)), \quad (2)$$

and with y, u respectively the output and input signal of the plant.

The (asymptotic) limiting parameter estimate θ^* [16] is defined according to

$$\theta^* = \arg \min_{\theta} \lim_{N \rightarrow \infty} \mathbb{E} [V_N(\theta, Z^N)],$$

with $\mathbb{E}[\cdot]$ the expectation operator.

The measurement data is assumed to be generated according to ³

$$y(t) = G_0(q)u(t) + v(t) \quad (3)$$

where $G_0(q)$ a linear time-invariant dynamical system, $u(t)$ is a measured input sequence, and $v(t)$ denotes an additional unknown contribution to $y(t)$. It is assumed that $v(t) = H_0(q)e(t)$ with H_0 a linear time-invariant monic stable filter, and e a stationary stochastic zero-mean white noise process. Moreover v is considered to be uncorrelated with the input signal u . Furthermore, we denote by \mathcal{M} the set of models $\{G(q, \theta), H(q, \theta)\}_{\theta \in \Theta}$ and by \mathcal{G} the set of plant models $\{G(q, \theta)\}_{\theta \in \Theta}$ with Θ representing the particular range of parameters determining the model sets, typically $\Theta \subset \mathbb{R}^d$. Throughout this paper the input signal is considered to be a known -deterministic- signal, that may have been generated as one particular realization of a stochastic process. This implies that the expectation operator \mathbb{E} refers to the random process v only.

For purpose of analysis, the residual signal $\varepsilon(t, \hat{\theta}_N)$ related to the estimated parameter $\hat{\theta}_N$ (1) is decomposed as:

$$\varepsilon(t, \hat{\theta}_N) = \beta_b(t, \hat{\theta}_N, G_0, \theta^*) + \beta_v(t, \hat{\theta}_N, \theta^*) + \varepsilon_v(t, \hat{\theta}_N) \quad (4)$$

with

$$\beta_b(t, \hat{\theta}_N, G_0, \theta^*) = H^{-1}(q, \hat{\theta}_N)[G_0(q)u(t) - G(q, \theta^*)u(t)] \quad (5)$$

$$\beta_v(t, \hat{\theta}_N, \theta^*) = H^{-1}(q, \hat{\theta}_N)[G(q, \theta^*)u(t) - G(q, \hat{\theta}_N)u(t)] \quad (6)$$

$$\varepsilon_v(t, \hat{\theta}_N) = H^{-1}(q, \hat{\theta}_N)v(t) \quad (7)$$

such that

- i. $\beta_b(t, \hat{\theta}_N, G_0, \theta^*)$ corresponds to that part of the residual signal that is induced by the asymptotic bias of the estimated model $G(q, \theta^*)$.

³ The effect of possible non-zero initial conditions is not incorporated here since it does not contribute essentially to the discussion at hand.

- ii. $\beta_v(t, \hat{\theta}_N, \theta^*)$ is the component in $\varepsilon(t, \hat{\theta}_N)$ that is induced by the variance error in the parameter estimate $G(q, \hat{\theta}_N)$ with respect to $G(q, \theta^*)$.
- iii. $\varepsilon_v(t, \hat{\theta}_N)$ corresponds to the effect of measurement noise $v(t)$, and additionally represents modelling errors in the estimated noise model $H(q, \hat{\theta}_N)$.

Assume that the measurements $\{y, u\}_N$ are generated according to expression (3). For a given estimated model $G(q, \hat{\theta}_N)$ the residual signal $\varepsilon(t, \hat{\theta}_N)$ is then given by expression (4). In this setting, the model structure validation problem is formulated as the problem of evaluating the hypothesis

$$\Upsilon_0 : \beta_b(t, \hat{\theta}_N, G_0, \theta^*) = 0.$$

Under persistence of excitation conditions on the input signal, this hypothesis is equivalent to the hypothesis that θ^* satisfies $G(q, \theta^*) = G_0(q)$, also referred to as $\theta^* = \theta_0$.

The hypothesis test is also directly related to the question whether the chosen model structure is rich enough to contain the true system. In this respect a distinction has to be made between different model structures. For model structures with independent parametrizations of $G(q, \theta)$ and $H(q, \theta)$ (e.g. Output error and Box Jenkins model structures) hypothesis Υ_0 becomes equivalent to $G_0 \in \mathcal{G}$. For dependently parametrized structures (e.g. ARX and ARMAX), Υ_0 is equivalent to $(G_0, H_0) \in \mathcal{M}$, since for these latter structures it is impossible to have $G(q, \theta^*) = G_0(q)$ without having $H(q, \theta^*) = H_0(q)$.

When Υ_0 holds the residual signal $\varepsilon(t, \hat{\theta}_N)$ in (4) reduces to

$$\varepsilon(t, \hat{\theta}_N) = \beta_v(t, \hat{\theta}_N, \theta_0) + \varepsilon_v(t, \hat{\theta}_N) =: \xi_v(t, \hat{\theta}_N), \quad (8)$$

in the sequel to be referred to as $\xi_v(t, \hat{\theta}_N)$.

In the next section we will introduce and analyze a test statistic for this hypothesis test on the basis of the sample cross-correlation function

$$\hat{R}_{\varepsilon u}(\tau) := \frac{1}{N} \sum_{t=1}^N \varepsilon(t, \hat{\theta}_N) u(t - \tau), \quad (9)$$

for $\tau = 0, \dots, n_\tau - 1$ and n_τ a user's choice.

For ease of notation we will denote the vectors

$$\begin{aligned} \hat{\mathbf{R}}_{\varepsilon u} &:= [\hat{R}_{\varepsilon u}(0) \cdots \hat{R}_{\varepsilon u}(n_\tau - 1)]^T \\ \hat{\mathbf{R}}_{\xi_v u} &:= [\hat{R}_{\xi_v u}(0) \cdots \hat{R}_{\xi_v u}(n_\tau - 1)]^T. \end{aligned}$$

Similarly for the residual signals:

$$\varepsilon(\hat{\theta}_N) := [\varepsilon(1, \hat{\theta}_N) \cdots \varepsilon(N, \hat{\theta}_N)]^T \quad (10)$$

$$\xi_v(\hat{\theta}_N) := [\xi_v(1, \hat{\theta}_N) \cdots \xi_v(N, \hat{\theta}_N)]^T, \quad (11)$$

and accordingly for $\varepsilon_v(\hat{\theta}_N)$, $\varepsilon(\theta^*)$ and $\varepsilon_v(\theta^*)$. $R_{\varepsilon\varepsilon}(\tau)$ will be denoted by $R_\varepsilon(\tau)$.

3 Cross-correlation test statistic and its analysis

3.1 Introduction

Suppose that a model structure has been chosen and that, for this model structure, the parameter estimate (1) has been obtained. For testing the hypothesis Υ_0 a test statistic will be used that is based on the sample cross-correlation function $\hat{\mathbf{R}}_{\varepsilon u}$. More specifically it will be tested whether this sample cross-correlation is likely to be a realization of the random vector $\hat{\mathbf{R}}_{\xi_v u}$. In order to verify this, we need to specify the statistical properties of $\hat{\mathbf{R}}_{\xi_v u}$. This will be done in two steps: first deriving an expression for $\varepsilon(\hat{\theta}_N)$ in terms of $\varepsilon(\theta^*)$. Subsequently an expression for ξ_v and the statistics of $\hat{\mathbf{R}}_{\xi_v u}$ will be derived.

3.2 General expression for $\varepsilon(\hat{\theta}_N)$

Consider that in a neighborhood of $\theta = \hat{\theta}_N$,

$$\varepsilon(t, \theta) \approx \varepsilon(t, \hat{\theta}_N) + \left. \frac{\partial \varepsilon(t, \theta)}{\partial \theta} \right|_{\theta=\hat{\theta}_N} (\theta - \hat{\theta}_N). \quad (12)$$

Using the definition $\psi(t, \hat{\theta}_N) = - \left. \frac{\partial \varepsilon(t, \theta)}{\partial \theta} \right|_{\theta=\hat{\theta}_N}$, it follows that for $\theta = \theta^*$

$$\varepsilon(t, \hat{\theta}_N) \approx \varepsilon(t, \theta^*) - \psi^T(t, \hat{\theta}_N) (\hat{\theta}_N - \theta^*). \quad (13)$$

Consider also that, by (1), $V'_N(\hat{\theta}_N) = 0$ or equivalently

$$\frac{1}{N} \sum_{t=1}^N \psi(t, \hat{\theta}_N) \cdot \varepsilon(t, \hat{\theta}_N) = 0. \quad (14)$$

Substituting $\varepsilon(t, \hat{\theta}_N)$ from (13) then yields

$$\frac{1}{N} \sum_{t=1}^N \psi(t, \hat{\theta}_N) \left[\varepsilon(t, \theta^*) - \psi^T(t, \hat{\theta}_N) (\hat{\theta}_N - \theta^*) \right] = 0. \quad (15)$$

By using the vector notation

$$\Psi_{\hat{\theta}} = \begin{bmatrix} \psi^T(1, \hat{\theta}_N) \\ \vdots \\ \psi^T(N, \hat{\theta}_N) \end{bmatrix} \quad (16)$$

the parameter error $\hat{\theta}_N - \theta^*$ can be written in a linear regression-type form as:

$$\hat{\theta}_N - \theta^* = (\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}})^{-1} \Psi_{\hat{\theta}}^T \varepsilon(\theta^*). \quad (17)$$

Moreover (13) can be rewritten as

$$\varepsilon(\hat{\theta}_N) = \varepsilon(\theta^*) - \Psi_{\hat{\theta}}(\hat{\theta}_N - \theta^*) \quad (18)$$

which by substitution of (17) leads to

$$\varepsilon(\hat{\theta}_N) = [I - \Psi_{\hat{\theta}}[\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}}]^{-1} \Psi_{\hat{\theta}}^T] \varepsilon(\theta^*). \quad (19)$$

Note that this expression holds irrespective of the question whether Υ_0 holds or not.

3.3 Expression for ξ_v

Under hypothesis Υ_0 , $\xi_v(\hat{\theta}_N) = \varepsilon(\hat{\theta}_N)$, and $\varepsilon(\theta^*) = \varepsilon_v(\theta^*)$, so that (19) becomes

$$\xi_v(\hat{\theta}_N) = [I - \Psi_{\hat{\theta}}[\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}}]^{-1} \Psi_{\hat{\theta}}^T] \varepsilon_v(\theta^*). \quad (20)$$

This final expression for $\xi_v(\hat{\theta}_N)$ shows a nice and interesting structure. Except for the noise term $\varepsilon_v(\theta^*)$ it is directly computable from data, as for a given $\hat{\theta}_N$, $\Psi_{\hat{\theta}}$ is fully known. In expression (20) it is also immediate that the mapping from $\varepsilon_v(\theta^*)$ to $\xi_v(\hat{\theta}_N)$ is a projection operator, implying that the signal $\xi_v(t, \hat{\theta}_N)$ will always have a smaller power than the signal $\varepsilon_v(t, \theta^*)$. I.e. the variance error of the parameter estimate attracts part of the process noise that subsequently is not present anymore in the residual $\xi_v(\hat{\theta}_N)$.

Note that the analysis starting with (12) is slightly different from the classical one ([16,23]) where a Taylor approximation is considered on the cost function rather than on the residual, leading to an expression for ξ_v that contains expectation operators rather than directly computable expressions. The analysis presented here builds on alternative results on uncertainty quantification as presented in [6,8] and further expanded in [4].

3.4 Statistical properties of $\hat{\mathbf{R}}_{\xi_v u}$

In order to specify the statistical properties of our test statistic $\hat{\mathbf{R}}_{\xi_v u}$, we write

$$\hat{\mathbf{R}}_{\xi_v u} = \frac{1}{N} \underbrace{\begin{bmatrix} u(1) & u(2) & \cdots & \cdots & u(N) \\ & \ddots & \cdots & \cdots & \vdots \\ & & u(1) & \cdots & u(N-n_\tau+1) \end{bmatrix}}_{P_u} \underbrace{\begin{bmatrix} \xi_v(1, \hat{\theta}_N) \\ \vdots \\ \xi_v(N, \hat{\theta}_N) \end{bmatrix}}_{\xi_v(\hat{\theta}_N)}.$$

By application of the asymptotic analysis that is commonly used in prediction error identification ([16], section 9.2)

$\hat{\mathbf{R}}_{\xi_v u}(\tau)$ will converge to a zero-mean Gaussian distribution asymptotically in N :

$$\hat{\mathbf{R}}_{\xi_v u} \rightarrow \mathcal{N}(0, P_{\Upsilon_0}/N) \quad (21)$$

with asymptotic covariance matrix

$$P_{\Upsilon_0} = \frac{1}{N} P_u \Lambda_{\xi_v(\hat{\theta}_N)} P_u^T \quad (22)$$

and $\Lambda_{\xi_v(\hat{\theta}_N)} = \mathbb{E}[\xi_v(\hat{\theta}_N) \xi_v^T(\hat{\theta}_N)]$.

The hypothesis test now verifies whether $\hat{\mathbf{R}}_{\xi_v u}$ is likely to be a realization of the random variable $\hat{\mathbf{R}}_{\xi_v u}$

$$\Upsilon_0 \text{ is true} \implies \hat{\mathbf{R}}_{\xi_v u}^T P_{\Upsilon_0}^{-1} \hat{\mathbf{R}}_{\xi_v u} \in \chi^2(n_\tau) \quad (23)$$

and the hypothesis is unfalsified if

$$\hat{\mathbf{R}}_{\xi_v u}^T P_{\Upsilon_0}^{-1} \hat{\mathbf{R}}_{\xi_v u} \leq c_\chi(\alpha, n_\tau), \quad (24)$$

with $c_\chi(\alpha, n_\tau)$ corresponding to the $1 - \alpha$ quantile of the χ^2 -distribution with n_τ degrees of freedom, i.e. for $x \in \chi^2(n_\tau) \implies \Pr(x \leq c_\chi(\alpha, n_\tau)) = \alpha$, and the covariance matrix P_{Υ_0} is given by expression (22).

By utilizing expression (20) the covariance matrix (22) can be approximated by

$$\hat{P}_{\Upsilon_0} = \frac{1}{N} P_u [I - \Psi_{\hat{\theta}}[\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}}]^{-1} \Psi_{\hat{\theta}}^T] \Lambda_{\varepsilon_v(\theta^*)} [\cdot]^T P_u^T \quad (25)$$

$$\Lambda_{\varepsilon_v(\theta^*)} = \mathbb{E}[\varepsilon_v(\theta^*) \varepsilon_v^T(\theta^*)]. \quad (26)$$

In a practical situation $\Lambda_{\varepsilon_v(\theta^*)}$ has to be estimated from data (see Section 4). The approximation \hat{P}_{Υ_0} is formally only exact in the case where $\Psi_{\hat{\theta}}$ is deterministic, which holds e.g. for Output Error model structures with linearly parametrized orthogonal basis functions models [12]. Note that in this situation due to the linear parametrization, the Taylor approximation (13) is also exact. By following a reasoning as presented in Proposition 1 in [7,8], it can be motivated that the χ^2 test statistic with \hat{P}_{Υ_0} remains reliable also for other model structures, under the condition that $V^T \varepsilon_v(\theta^*)$ converges to a Gaussian distribution⁴ fast enough, where V is a unitary matrix determined by the singular value decomposition

$$I - \Psi_{\hat{\theta}}[\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}}]^{-1} \Psi_{\hat{\theta}}^T = U \Sigma V^T.$$

Although V will generally also be non-deterministic, the latter condition seems to be less severe than the condition that underlies the classical result (21) and (22), that relies on asymptotic normality of $\xi_v(\hat{\theta}_N)$, in particular when $\varepsilon_v(\theta^*)$ is Gaussian distributed. These additional convergence properties are due to the new analysis presented here, and are not present in the classical results [16,23].

⁴ In this alternative reasoning actually an alternative test statistic $\hat{\mathbf{R}}_{\gamma_v u}$ with $\gamma_v = \Sigma^{-1} U^T \xi_v$ is used as a starting point that leads to a similar χ^2 -test.

4 Estimating noise properties

4.1 Which information is required?

In order to perform the statistical hypothesis test the noise covariance matrix $\Lambda_{\varepsilon_v(\theta^*)}$ (26) needs to be estimated from data. This involves the covariance information in the noise term

$$\varepsilon_v(t, \theta^*) = H(q, \theta^*)^{-1}v(t) \quad (27)$$

$$= H(q, \theta^*)^{-1}H_0(q)e(t). \quad (28)$$

The required information is dependent on the particular formulation of the hypothesis test that is considered. The following two situations can be distinguished:

- If the hypothesis Υ_0 is equivalent to $G_0 \in \mathcal{G}$ only (i.e. $G(q, \theta^*) = G_0(q)$), $\varepsilon_v(t, \theta^*)$ is given by (28), and an accurate estimate of H_0 and the noise variance σ_e^2 are required, while $H(q, \theta^*)$ is estimated by $H(q, \hat{\theta}_N)$.
- If the hypothesis Υ_0 is equivalent to $(G_0, H_0) \in \mathcal{M}$, (i.e. $G(q, \theta^*) = G_0(q)$ and $H(q, \theta^*) = H_0(q)$), $\varepsilon_v(t, \theta^*)$ reduces to $e(t)$, and by virtue of the whiteness of e , the necessary information to be determined from data is the noise variance σ_e^2 .

One important observation that can be made is that, in the first situation, even though there is no intention to verify whether $H(q, \theta^*) = H_0(q)$, an accurate estimate of the noise model H_0 should be available. This observation is in contrast with the often considered situation that the standard cross-correlation test can validate estimated models \hat{G} without explicitly estimating noise models. In other words: the potential of validating a process model \hat{G} without taking due care of estimating an appropriate noise model, is questionable. This will be further explored in subsequent sections.

4.2 Estimating noise dynamics

In the situation of a hypothesis that reflects $G(q, \theta^*) = G_0(q)$ the noise covariance $\Lambda_{\varepsilon_v(\theta^*)}$ needs to be estimated, with $\varepsilon_v(t, \theta^*) = H(q, \theta^*)^{-1}v(t)$. Since in the sequel $\varepsilon_v(t, \theta^*)$ will be approximated by $\varepsilon_v(t, \theta^*) \approx H^{-1}(q, \hat{\theta}_N)v(t)$, the noise covariance matrix $\Lambda_{\varepsilon_v(\theta^*)}$ can be computed by simply deriving the spectral properties of $v(t) = H_0(q)e(t)$, i.e. by deriving an estimated model of H_0 and an accurate estimate of the variance σ_e^2 of $e(t)$.

In order to construct these estimates, the main bottleneck is that the noise component in the data should be separated from the contribution of the input signal $u(t)$. Here we propose two different methods to achieve this.

The first method requires the use of a periodic (repeated) input signal. Consider two sets of measurement data $\{u, y_1\}$ and $\{u, y_2\}$, both generated with the same input u . With

expression (3) it holds that the difference $\varepsilon_d(t)$ between the two measured outputs can be written as⁵

$$\varepsilon_d(t) := \sqrt{2}[y_1(t) - y_2(t)] = \sqrt{2}[v_1(t) - v_2(t)]. \quad (29)$$

The difference signal $\varepsilon_d(t)$ qualifies for estimating the properties of the signal $v(t)$. Indeed, the difference signal $\varepsilon_d(t)$ does not contain terms related to the input u . Only some care has to be taken with the initial conditions, i.e. the effect of past input values.

From ε_d it is easy to estimate the required model of H_0 as a time-series model $H(q, \hat{\theta}_v)$ describing the dynamics of ε_d . Moreover, the required estimate of σ_e^2 can be obtained by $\hat{\sigma}_e^2 = \frac{1}{N} \sum_{t=1}^N [H(q, \hat{\theta}_v)^{-1}\varepsilon_d(t, \hat{\theta}_v)]^2$; in this procedure a parametric model structure and a proper model order selection procedure have to be selected for estimating $H(q, \hat{\theta}_v)$ (cf. the ARMASA toolbox of [2,1]).

In case the input signal is not a user's choice, accurate noise dynamics can be estimated by employing an auxiliary plant model $G_a(q, \hat{\theta}_a)$, estimated as an output error model with a model order high enough to be reasonably certain that the effects of undermodelling are negligible. Construct the residual signal $\varepsilon(t, \hat{\theta}_a)$ according to

$$\varepsilon(t, \hat{\theta}_a) = y(t) - G(q, \hat{\theta}_a)u(t).$$

With the earlier analysis, and with neglecting effects of undermodelling in $G(q, \hat{\theta}_a)$ it follows that

$$\varepsilon(t, \hat{\theta}_a) \approx \beta_v(t, \hat{\theta}_a, \theta_a^*) + v(t)$$

which in vector form is denoted as

$$\varepsilon(\hat{\theta}_a) \approx [I - \Psi_{\hat{\theta}_a} [\Psi_{\hat{\theta}_a}^T \Psi_{\hat{\theta}_a}]^{-1} \Psi_{\hat{\theta}_a}^T] v. \quad (30)$$

Whereas this latter expression gives the impression that v can be reconstructed from $\varepsilon(\hat{\theta}_a)$ this is not true, since the corresponding matrix $[I - \Psi_{\hat{\theta}_a} [\Psi_{\hat{\theta}_a}^T \Psi_{\hat{\theta}_a}]^{-1} \Psi_{\hat{\theta}_a}^T]$ appears to be singular. The following approach is now followed to construct a dynamic model for v :

- (1) Neglecting the projection operator in (30), the required model of H_0 can be determined by identifying a time series model $H(q, \hat{\theta}_v)$ describing the dynamics of the time series $\varepsilon(\hat{\theta}_a)$. Moreover, an intermediate estimate of σ_e^2 is obtained through $\hat{\sigma}_{e, \text{int}}^2 = \frac{1}{N} \sum_{t=1}^N [H(q, \hat{\theta}_v)^{-1}\varepsilon(t, \hat{\theta}_a)]^2$.
- (2) In a second step, the intermediate noise variance estimate is corrected in order to take into account the effect

⁵ The scaling with $\sqrt{2}$ is only applied to maintain the same signal variance.

of the projection operator in (30):

$$\hat{\sigma}_e^2 = \frac{N}{N - n_a} \hat{\sigma}_{e,int}^2 \quad (31)$$

with n_a the dimension of $\hat{\theta}_a$. The scaling factor in the latter equation is motivated by the fact that $\text{trace}[I - \Psi_{\hat{\theta}_a} [\Psi_{\hat{\theta}_a}^T \Psi_{\hat{\theta}_a}]^{-1} \Psi_{\hat{\theta}_a}^T] = N - n_a$. It implies that, although the dynamic information on v is obtained from $\varepsilon(t, \hat{\theta}_a)$, its variance is corrected for by using the relation (30).

Note that this method does suffer from the fact that the noise model $H(q, \hat{\theta}_v)$ is based on the properties of $\varepsilon(t, \hat{\theta}_a)$ rather than $v(t)$ itself. Important is the fact that the variance is estimated consistently, provided that $\hat{\theta}_v$ is consistent, a proof of which can be found in [16, p. 471]. Finally, note that the auxiliary model can be a very poor model from a variance point of view; the variance in the model is of no consequence for the purpose of estimating the variance of v consistently.

Other approaches to the estimation of noise properties in case of undermodelling are suggested in [24],[14] and [20]. In [24] the use of high order models for noise variance estimation is also suggested. The estimation procedure applied there is based on bootstrapping. The effect of modelling part of the noise into the model is not taken into account in that paper. In [20] an alternative method is given for providing a non-parametric estimate of the noise dynamics in $v(t)$, without the necessity of estimating an accurate parametric plant model.

5 Comparison with the standard cross-correlation test

The cross-correlation test as implemented in the Identification Toolbox in Matlab will be referred to as the *standard cross-correlation test* [17]. Like the test presented in the previous section it is based on the sample cross-correlation $\hat{R}_{\varepsilon u}(\tau)$ between $u(t)$ and $\varepsilon(t, \hat{\theta}_N)$, and states that an estimated model $\hat{\theta}_N$ is not invalidated if the sequence $\hat{R}_{\varepsilon u}(\tau)$ satisfies

$$|\hat{R}_{\varepsilon u}(\tau)| < \gamma(\alpha), \quad \text{for } |\tau| \leq n_\tau - 1, \quad \text{with} \quad (32)$$

$$\gamma(\alpha) = c_{\mathcal{N}}(\alpha) \sqrt{\frac{P_1}{N}} \quad (33)$$

$$P_1 = \sum_{\kappa=-n_\tau+1}^{n_\tau-1} \hat{R}_u(\kappa) \hat{R}_\varepsilon(\kappa) \quad (34)$$

$$\text{where } \hat{R}_\varepsilon(\kappa) = \frac{1}{N} \sum_{t=1}^N \varepsilon(t, \hat{\theta}_N) \varepsilon(t - \kappa, \hat{\theta}_N) \quad (35)$$

and $\hat{R}_u(\kappa)$ accordingly, and where $c_{\mathcal{N}}(\alpha)$ is the $1 - \alpha$ quantile of the Gaussian distribution $\mathcal{N}(0, 1)$, i.e. for $x \in \mathcal{N}(0, 1) \implies \Pr(x \leq c_{\mathcal{N}}(\alpha)) = \alpha$, and where the probability level α and the number of considered lags n_τ are user's

choices. This correlation test is actually based on the hypothesis that $\varepsilon(t, \hat{\theta}_N)$ and u are uncorrelated, which actually comes down to testing the hypothesis

$$\Upsilon_1 : \beta_b(t, \hat{\theta}_N, G_0, \theta^*) + \beta_v(t, \hat{\theta}_N, \theta^*) = 0$$

which under persistency of excitation conditions on the input signal becomes equivalent to the expression $\hat{\theta}_N = \theta_0$, rather than $\theta^* = \theta_0$, as is the case in the analysis of the earlier sections. This implies that the test basically neglects any random effect in the estimated parameter, by assuming that $\varepsilon(t, \hat{\theta}_N) = \varepsilon_v(t, \hat{\theta}_N)$.

While P_{Υ_0} corresponds to hypothesis Υ_0 , the (covariance) matrix that formally corresponds to the hypothesis test Υ_1 is given by

$$P_{\Upsilon_1} = \frac{1}{N} P_u \Lambda_{\varepsilon_v(\theta^*)} P_u^T, \quad (36)$$

and that the applied covariance P_1 is actually an estimate of the (1, 1) entry of

$$\frac{1}{N} P_u \Lambda_{\varepsilon(\hat{\theta}_N)} P_u^T \quad (37)$$

(see [4] for a full analysis.)

The major differences with the validation test presented in Section 3 can now be summarized as follows:

- (a) The standard cross-correlation test is only point-wise. This means that the correlation between the terms of $\hat{R}_{\varepsilon u}(\tau)$ over lags τ is not taken into consideration. The first consequence is that the interpretation of the false alarm rate $(1 - \alpha)$ remains unclear. A second consequence is that many models with an undermodelling error will not be invalidated by the test as the correlation in $\hat{R}_{\varepsilon u}(\tau)$, may be hidden in the pointwise evaluation. See, e.g. the example in the next section.
- (b) The standard test applied a different and rather awkward hypothesis test (Υ_1) that actually neglects any random effect in the estimated parameters. This translates to a covariance matrix P_{Υ_1} (36) that in comparison with P_{Υ_0} (25) lacks a projection mechanism.
- (c) When considering P_1 as an estimate of the (1,1) element of the covariance matrix P_{Υ_1} , it appears that $\Lambda_{\varepsilon(\hat{\theta}_N)}$ is used as an estimate of $\Lambda_{\varepsilon_v(\theta^*)}$. This implies that for the diagonal elements of this matrix that

$$\hat{R}_{\varepsilon_v(\theta^*)}(0) = \frac{1}{N} \sum_{t=1}^N \varepsilon^2(t, \hat{\theta}_N). \quad (38)$$

However expression (4) immediately reveals the problem which occurs when doing so. Indeed, from expressions

(4),(8) it follows that

$$\hat{R}_{\varepsilon_v(\theta^*)}(0) \approx \frac{1}{N} \sum_{t=1}^N [\beta_b^2(t, \hat{\theta}_N, G_0, \theta^*) + \xi_v^2(t, \hat{\theta}_N)] \quad (39)$$

where the cross terms are neglected since they tend to 0 for increasing values of N , provided that u and v are uncorrelated. For low model orders n (with respect to G_0) the residual sequence $\varepsilon(t, \hat{\theta}_N)$ contains a large undermodelling contribution $\beta_b(t, \hat{\theta}_N, G_0, \theta^*)$ causing an offset in the estimate (38). On the other hand, while for large model orders n the undermodelling contribution will be small, a part of the measurement noise $v(t)$ is modelled in the parameter $\hat{\theta}_N$ and as such does not appear in the residuals as reflected in the term $\xi_v(t, \hat{\theta}_N)$, which with expression (19) is quantified as

$$\frac{1}{N} \sum_{t=1}^N \xi_v^2(t, \hat{\theta}_N) = \frac{1}{N} \left\| [I_N - \Psi_{\hat{\theta}} [\Psi_{\hat{\theta}}^T \Psi_{\hat{\theta}}]^{-1} \Psi_{\hat{\theta}}^T] \varepsilon_v(\theta^*) \right\|_2^2.$$

In fact, for $n = N$ the residual error $\varepsilon(t, \hat{\theta}_N)$ is zero as the noise is completely modelled. This shows that the residual error $\varepsilon(t, \hat{\theta}_N)$ cannot be considered to be representative for $\varepsilon_v(\theta^*)$ without due care. This is even more so when also dynamical properties of the noise need to be estimated, as e.g. $R_{\varepsilon_v(\theta^*)}(\tau)$ for lags other than zero; the (unknown) dynamic behaviour of the undermodelling term $\beta_b(t, \hat{\theta}_N, G_0, \theta^*)$ and the term $\xi_v(t, \hat{\theta}_N, \theta^*)$ then distort the correlation in the signal $\varepsilon(t, \hat{\theta}_N)$. This latter situation shows that in estimating the noise characteristics, the classical cross-correlation test actually assumes that $\beta_b + \beta_v = 0$, and therefore the test appears to be valid only under the assumptions that it intends to validate.

6 Illustrative example

In order to illustrate the results from the previous sections, we consider the following simulation example. There are $N = 256$ measurements $\{y, u\}_N$ generated according to $y(t) = G_0(q)u(t) + v(t)$ with $u(t)$ and $v(t)$ white noise sequences with variances $\sigma_u^2 = 1$ and $\sigma_v^2 = 0.09$, respectively, and with the true system

$$G_0(q) = \frac{0.01293q^{-1} + 0.1062q^{-2} + 0.1058q^{-3} + 0.01279q^{-4}}{1 - 0.2482q^{-1} + 1.091q^{-2} - 0.2441q^{-3} + 0.9822q^{-4}}.$$

Note that the input signal is considered known and deterministic. Output Error (OE) models of orders 1 to 10 are estimated from this data, through the model structure

$$G_n(q, \theta) = \frac{q^{-1} \sum_{k=0}^{n-1} b_k q^{-k}}{1 + \sum_{k=1}^n f_k q^{-k}} \text{ for } n = [1, 10] \quad (40)$$

and noise model $H(q, \theta) = 1$, leading to estimated plant models $\hat{G}_n(q)$.

Figure 1 shows the frequency response of the fourth order system G_0 and of the second order model $\hat{G}_2(q)$, while the latter model is accompanied by an uncertainty region corresponding to a 99% probability level. Due to the limited model order the second resonance peak of the system is not contained in the identified model. Applying the standard cross-correlation test between model residuals and input, as present in Matlab's System Identification Toolbox, shows that the sample cross-correlation function between the residuals of the OE-model and the input remains within the standard test-bounds depicted in solid lines of Figure 1(c). In other words, the standard cross-correlation test does not invalidate the second order OE-model, and the related 99% model uncertainty bounds that are based on the presumed assumption that there are variance errors only (system is in the model class), fails to contain the true system. In or-

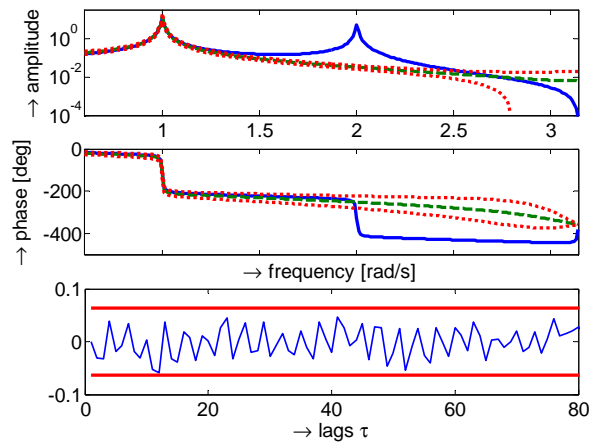


Fig. 1. (a)-(b):Bode-plots of a fourth order system $G_0(q)$ (solid blue), a second order OE-estimate (dashed green) and the standard 99% variance-based confidence bounds of the second order OE-estimate (dotted red). Figure (c) depicts the standard cross-correlation test $\hat{R}_{\varepsilon u}(\tau) := \frac{1}{N} \sum_{t=1}^N \varepsilon(t, \hat{\theta}_N)u(t - \tau)$ with the standard 99% confidence bound (solid red).

der to check whether undermodelling could have been detected easily by other means, the transfer function from $u(t)$ to $\varepsilon(t, \hat{\theta}_N)$ is estimated using the approach of Model Error Modelling [15]. Figure 2 shows the frequency response of a high order FIR (Model Error) Model identified from input to residual signal. The 99% uncertainty interval around 0 contains the Model Error Model, from which it is generally concluded that there is no statistical indication that there is an undermodelling error. As a final test to detect whether we could have recognized any unmodelled dynamics from the measurement data, an Empirical Transfer Function Estimate (ETF) is calculated from the measurement data, as sketched in Figure 3. This result shows that it is hard to detect the unmodelled resonance peak, as it is completely hidden in the noise that is present. Figure 4.c shows the

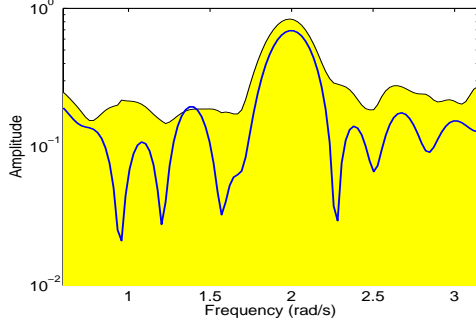


Fig. 2. Frequency response of a high order FIR (Model Error) Model from input to residual signal of the second order OE model as provided by Matlab's System Identification Toolbox [17], together with its 99% uncertainty bound around 0 (shaded in yellow).

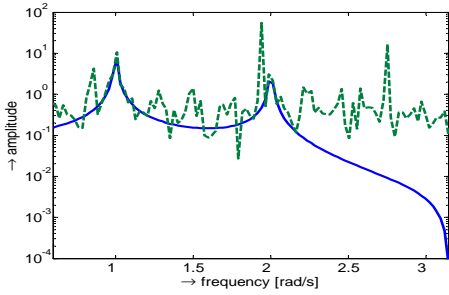


Fig. 3. Frequency response of the true system (solid blue) and the ETFE estimate (dashed green).

undermodelling component $\hat{R}_{\beta_b u}(\tau)$ that is present in the cross-correlation $\hat{R}_{\epsilon u}(\tau)$. Note the structural behaviour of this term, reflecting the unmodelled resonance peak. Note also that in a real identification experiment the signal β_b is of course not available. In Figure 4.b. the actual noise contribution $\hat{R}_{\epsilon_v u}(\tau)$ is compared with the bound $\gamma(\alpha)$ of the classical test (see (33)). $\gamma(\alpha)$ is supposed to be an upper-bound on $R_{\epsilon_v u}$, however the bound is clearly overestimating the noise contribution, which is due to the incorporation of the undermodelling terms itself in the estimation of the variance, by using expression (38), as well as by neglecting the parameter variance term β_v (projection mechanism).

Next, the method as presented in Section 3-4 will be applied. For this purpose the noise dynamics are estimated by using the second method of Section 4. A time series model is estimated with the ARMASA-toolbox on the residuals of an OE-model of order $N/5$ (which is extreme to show the potential of the method) and the noise variance is estimated according to (31). New bounds (dashed-dotted black) are obtained. These new bounds are not corrupted by undermodelling effects and as such they are tighter bounds for the noise contribution (cf. Figure 4.b.) Figure 5 depicts the results of the new (vector-valued) test. The curves depict the test value $\hat{\mathbf{R}}_{\epsilon u}^T P^{-1} \hat{\mathbf{R}}_{\epsilon u}$, for $\hat{\mathbf{R}}_{\epsilon u} \in \mathbb{R}^{n_\tau}$ and for different choices of P . The test value should be smaller than the bound $c_\chi(\alpha, n_\tau)$ for the model not to be invalidated (cf. ex-

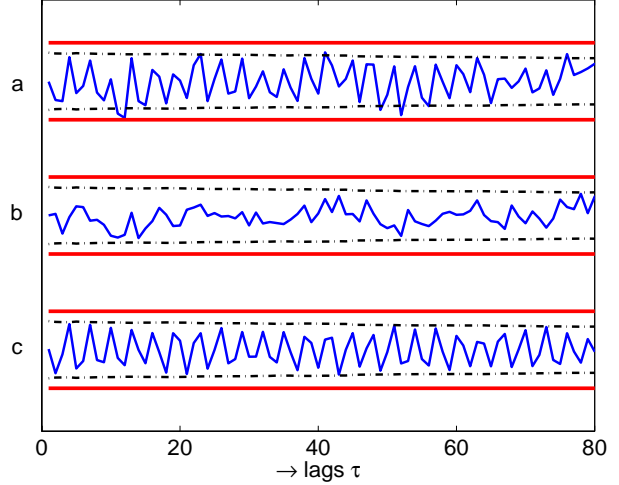


Fig. 4. The standard cross-correlation test applied to the OE-estimate $\hat{G}_2(q)$.

a: the sample cross-correlation $\hat{R}_{\epsilon u}(\tau)$ for lags $\tau = [0, 80]$;
b: the actual noise-contribution $\hat{R}_{\epsilon_v u}(\tau)$;
c: the undermodelling contribution $\hat{R}_{\beta_b u}(\tau)$ in $\hat{R}_{\epsilon u}(\tau)$.
The bounds $\gamma(\alpha)$ of the standard test (33) for $\alpha = .99$ are given in solid red and the newly proposed bounds in dashed black.

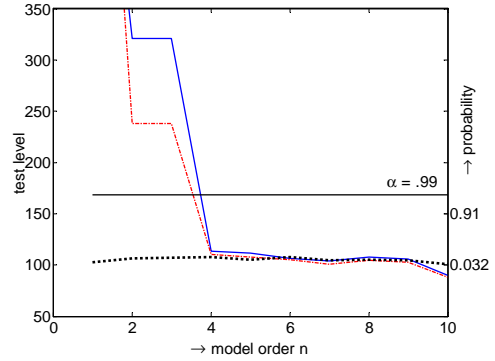


Fig. 5. The vector-valued cross-correlation test evaluated for the vector $\hat{\mathbf{R}}_{\epsilon u} \in \mathbb{R}^{128}$ of the first $N/2$ lags of the sample cross-correlation of an OE-model of increasing order $n = [1, 10]$. The test value $\hat{\mathbf{R}}_{\epsilon u}^T P^{-1} \hat{\mathbf{R}}_{\epsilon u}$ is compared with the bound $c_\chi(.99, 128)$ corresponding to the χ^2 -distribution of order $N/2$; values below the bound imply that the model is not invalidated. P is based on the true noise covariance (solid blue curve), on the sample covariance estimate (34)-(35) (dotted black curve), and on the covariance estimate according to Section 4 (dashed-dotted red curve).

pression (24)), against a false-alarm rate of $(1 - \alpha) \times 100\%$. The blue solid line depicts the test value for $P = P_{Y_0}$ when using the true noise properties $\Lambda_{\epsilon_v(\theta^*)}$ in the covariance matrix P_{Y_0} . The correct model order of four is easily identified from the graph as the smallest model order for which the test value becomes smaller than the bound ($\alpha = .99$). When replacing the noise covariance $\Lambda_{\epsilon_v(\theta^*)}$ by an estimate by following the procedure of Sections 3-4 the test levels differ from the actual levels, but the model orders are still properly

evaluated (red dashed-dotted line). When estimating $\Lambda_{\varepsilon_v(\theta^*)}$ by the residual covariance $\Lambda_{\varepsilon(\hat{\theta}_N)}$ (cf. expression (35)) the undermodelling errors are incorporated in the covariance estimate and a vector-valued cross-correlation test would let all model orders (1 to 10) pass (dotted black curve).

This example is also used in [21] where model validation issues are discussed when the input signal is not as exciting as white noise, and the second resonance peak is absent in the identified model due to a limited bandwidth of the input signal.

7 Validation data versus identification data

It is often suggested that the model validation test should be applied to validation data rather than to the same data that has been used for parameter estimation. In the standard test this is motivated by observing that the estimator (38) of the noise variance $R_{\varepsilon_v(\theta^*)}(0)$ under assumption $\theta^* = \theta_0$ can be written as

$$\hat{R}_{\varepsilon_v(\theta^*)}(0) = \frac{1}{N} \|\xi_v(\hat{\theta}_N)\|_2^2, \quad (41)$$

and that according to (20) this estimator has been shown to underestimate the real variance of $\varepsilon_v(t, \theta^*)$ for large model orders.

In the new test as presented in Section 3 one could replace the original hypothesis $\Upsilon_0 : \beta_b = 0$, by an alternative $\Upsilon_v : \beta_{b, val} = 0$, where $\beta_{b, val}$ is evaluated on validation data rather than on estimation data. This would lead to an alternative expression for the covariance matrix P_{Υ_v} , but does not seem to contribute to any improvement of the test. The major consequence of using validation data is that the number of data that is available for the test is reduced, thereby increasing the variance of the estimated models.

Referring back to the classical argument of using validation data for estimation of $R_{\varepsilon_v(\theta^*)}(0)$, consider the residual over the validation data set⁶:

$$\varepsilon_{val}(t, \hat{\theta}_N) = \beta_{b, val}(t) + \beta_{v, val}(t) + \varepsilon_{v, val}(t)$$

with the several terms defined in accordance with (4)-(7), replacing $u(t)$ by $u_{val}(t)$, and $v(t)$ by $v_{val}(t)$:

$$\beta_{b, val}(t) = H(q, \hat{\theta}_N)^{-1} [G_0 - G(\theta^*)] u_{val}(t) \quad (42)$$

$$\beta_{v, val}(t) = H(q, \hat{\theta}_N)^{-1} [G(\theta^*) - G(\hat{\theta}_N)] u_{val}(t) \quad (43)$$

$$\varepsilon_{v, val}(t) = H(q, \hat{\theta}_N)^{-1} v_{val}(t). \quad (44)$$

Under the hypothesis Υ_0 (implying $G(q, \theta^*) = G_0(q)$) and assuming that u_{id} and u_{val} have the same properties, it follows that

$$\frac{1}{N} \sum_{t=1}^N \varepsilon_{val}(t, \hat{\theta}_N)^2 = \quad (45)$$

$$= \frac{1}{N} \|\varepsilon_{v, val}(\hat{\theta}_N) - [\Psi_{val}(\Psi_{id}^T \Psi_{id})^{-1} \Psi_{id}^T] \varepsilon_{v, id}(\theta^*)\|_2^2, \quad (46)$$

⁶ Arguments of variables are simplified for ease of readability

where use has been made of relations (17),(18). If $\varepsilon_{v, id}$ and $\varepsilon_{v, val}$ are uncorrelated (as is usually assumed), then

$$\begin{aligned} \frac{1}{N} \sum_{t=1}^N \varepsilon_{val}(t, \hat{\theta}_N)^2 &= \frac{1}{N} \|\varepsilon_{v, val}(\hat{\theta}_N)\|_2^2 + \\ &+ \frac{1}{N} \|[\Psi_{val}(\Psi_{id}^T \Psi_{id})^{-1} \Psi_{id}^T] \varepsilon_{v, id}(\theta^*)\|_2^2. \end{aligned}$$

If we restrict to Output Error models, and to input signals that are the same in the identification and the validation data, then under the assumption of white noises ε_v in both identification and validation data, (i.e. the underlying system also has an Output Error structure) it follows that

$$R_{\varepsilon_{val}(\hat{\theta}_N)}(0) = \sigma_e^2 \frac{N+n}{N} \quad (47)$$

with n the dimension of $\hat{\theta}_N$.

This brings us to the following observations:

- In absence of model bias, using validation data to estimate the noise variance through the estimator (45) overestimates the noise variance with a quantity that is similar to the underestimation of the noise variance that occurs when applying (41) to estimation data.
- Both under-estimation and over-estimation can be corrected for, by taking account of the analysis results (20) for estimation data and (47) for validation data.
- If there is model bias, the bias component β_b will appear similarly in the estimation and the validation residual.
- Reserving data only for validation purposes reduces the number of data available for parameter estimation, and therefore yields larger parameter variance.

As a result, in the linear time-invariant systems framework as considered here, the use of validation data does not appear to provide any advantages over the use of identification data. It seems that using validation data in the standard model validation test is a poorly motivated instrument to work around overfitting of an estimated model, which actually can be treated more effectively by accurate noise modelling and accounting for the parameter variance.

8 Conclusions

The standard cross-correlation test works very well as a model structure validation test in many practical situations. However significant undermodelling errors can remain undetected. In this paper, a vector-wise correlation test is analysed that incorporates new and simple computational expressions for quantifying the variance contributions in estimated models. It is concluded that appropriate noise modelling is indispensable for accurate model structure validation and this shows the limitations of separate validation of plant and noise models, as e.g. applied in Output Error model structure validation. Finally it is argued that rather than reserving

part of the measurement data for validation purposes only, it is more attractive to avoid overfitting of identified models by accurate noise modelling and accounting for the parameter variance.

Even if the correlation-type validation test would be perfectly able to detect undermodelling in an estimated model, it should be stressed that data-based validation methods are principally limited to detect unmodelled dynamics only with respect to the current experimental data.

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