Correlation Based Model Validity Tests for Nonlinear Models

by

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Abstract

Correlation based model validity tests are derived which detect omitted linear and nonlinear dynamic terms in estimated models.

Introduction

Model validation should form the final stage of any identification procedure. If the system under analysis is linear then a number of well established tests are available for validating the estimated model [Goring & Unbehauen 1973, Boom & Enden 1973]. It can however easily be shown [Billings and Voon 1983] that the well known covariance tests which consist of computing the autocorrelation function of the residuals and the cross-correlation between the residuals and the input [Box and Jenkins 1976] which were developed for linear systems provide incorrect information whenever nonlinear effects [Billings 1980] are present in the data. Application of these tests may therefore mislead the experimenter into believing his model is adequate when it is not and new tests which overcome these deficiencies are required.

In the present study higher order correlation functions are introduced to detect the presence of unmodelled linear and nonlinear terms in the residuals. The results represent an extension of previous work [Billings and Fakhouri 1982, Billings and Voon 1983], which developed tests to indicate if the residuals were unpredictable from all linear and nonlinear combinations of past inputs and outputs. These tests however can only be applied when a noise model is estimated. Additional tests are required when instrumental variables or suboptimal least squares type algorithms [Billings and Voon 1984] are applied which yield unbiased estimates of the process model without estimating a noise model. Simple to compute and interpret tests which can be used in conjunction with these latter algorithms are introduced in the present study.

Problem Statement

It will be assumed throughout that the system under investigation is analytic and can be represented by a Volterra series

$$z(t) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \ldots \int h_n(\tau_1,\tau_2,\ldots\tau_n) \prod_{i=1}^{n} u(t-\tau_i)d\tau_i + e(t) \qquad (1)$$

Using the operator calculus developed by Brilliant and George [Billings 1980] eqn (1) can be expressed as

$$z(t) = \sum_{n=1}^{\infty} H_n\left[u(t)\right] + e(t) = \mathcal{H}\left[u(t)\right] + e(t)$$

$$= \sum_{n=1}^{\infty} H_n(u^n(t)) + e(t) \qquad (2)$$

where the square brackets indicate that H operates on u(t) and the parenthesis depict the actual relationship. It is important to emphasise that the continuous time Volterra series model is chosen as a convenient representation for a wide class of nonlinear systems. The fact that all the results are derived for this model does not constrain the applicability of the results to Volterra models only. The final results can be applied to all analytic nonlinear systems whatever form of model is used to characterise the input/output map.

The first stage in the analysis of any data ought to involve some simple calculations which indicate if the system under test is linear or nonlinear. There are several simple tests which yield this information.

Wherever the input $u(t)+b$, $\overline{u(t)} = 0$, $b \neq 0$ is applied to a system the system cannot be linear if $\overline{z_b(t)} \neq \overline{z(t)}$ where $\overline{z_b(t)}$ and $\overline{z(t)}$ are the mean levels of the system output for the inputs b (i.e. $u(t) = 0$)

and u(t)+b respectively. Alternatively, for an input u(t)+b, $b \neq 0$ where the third order moments of u(t) are zero and all even order moments exist (a sine wave, gaussian or ternary sequence would for example satisfy these conditions) then the process is linear iff [Billings and Voon 1983, Haber 1985]

$$\phi_{z'z'^2}(\tau) = E\{(z(t-\tau)-\bar{z})(z(t)-\bar{z})^2\} = 0 \;\forall \tau \qquad (3)$$

If the input u(t) for an excitation u(t)+b, $b \neq 0$ belongs to the separable class of random processes [Billings and Fakhouri 1982] then the system under test is linear iff

$$\phi_{u^2 z'}(\tau) = E\{(u(t-\tau))^2(z(t)-\bar{z})\} = 0 \;\forall \tau \qquad (4)$$

Examples of the application of all these tests are available in the literature.

The application of any of the above structure detection tests will indicate to the experimenter at an early stage in the analysis if it is worthwhile fitting a nonlinear model. Once a model of the process has been estimated, whether linear or nonlinear, model validity tests are applied to detect if there are any unmodelled terms in the residuals which if omitted from the model will induce biased estimates.

Model Validity Tests

Linear Systems

If a system is linear $\overline{z_b(t)} = z(t)$, $\phi_{z'z'^2}(\tau) = 0$ or $\phi_{u^2z'}(\tau) = 0$ then two simple covariance tests can be applied to detect unmodelled linear terms in the residuals [Box and Jenkins 1976]. If the process and the noise model estimates are correct then it can be shown that

$$\begin{aligned} \phi_{\xi\xi}(\tau) &= \delta(\tau) \\ \phi_{u\xi}(\tau) &= 0 \;\forall \tau \end{aligned} \qquad (5)$$

where $\xi(t)$ represents the residual sequence. If the process model is correct but the noise model is incorrect then the residuals will be autocorrelated $\phi_{\xi\xi}(\tau) \neq \delta(\tau)$ but they will be uncorrelated with the input $\phi_{u\xi}(\tau) = 0 \;\forall \tau$. Alternatively, if the noise model is correct and the process model is biased then the residuals are both autocorrelated $\phi_{\xi\xi}(\tau) \neq \delta(\tau)$ and correlated with the input $\phi_{u\xi}(\tau) \neq 0$. It is possible using these simple correlations therefore to distinguish between deficiencies in the process and the noise models.

The situation is not quite so straightforward when the system is nonlinear.

Nonlinear Systems

In nonlinear systems the noise may enter the system internally and cannot always be translated to be additive at the output [Leontaritis and Billings 1985]. The general situation, where noise e(t) possibly nonlinear, enters a nonlinear system internally can be represented by

$$z(t) = G^{u}\left[u(t)\right] + G^{ue}\left[u(t), e(t)\right] + G^{e}\left[\overset{e}{\cancel{u}}(t)\right] \tag{6}$$

where $G^{u}\left[u(t)\right]$, $G^{e}\left[e(t)\right]$ are functions of u(t) and e(t) only and $G^{ue}\left[u(t), e(t)\right]$ represents all cross-product terms. Since we have very little control over the form of the input signals and the residuals at the model validation stage we must derive tests which work under the worst possible combinations of signal properties. We will assume therefore that u(t) and e(t) are independent zero mean processes, all odd order moments are zero and $e(\cdot)$ is white and $u(\cdot)$ may be white.

Previous work has shown [Billings and Voon 1983] that every isolated term in eqn (6) if omitted from the model can be detected by three correlation tests. Specifically the residuals $\xi(t)$ will be unpredictable from all linear and nonlinear combinations of past inputs and outputs iff

$$\phi_{\xi\xi}(\tau) = \delta(\tau)$$
$$\phi_{u\xi}(\tau) = 0 \; \forall \tau$$
$$\phi_{\xi\xi u}(\tau) = E\left[\xi(t)\xi(t-1-\tau)u(t-1-\tau)\right] = 0 \quad \tau \geq 0 \tag{7}$$

Notice that the traditional tests used for linear systems eqn (6) are not sufficient.

The tests in eqn (7) can however only be applied if a noise model is fitted as part of the estimation procedure so that $\xi(t)$ is reduced to an unpredictable sequence. When instrumental variables (IV) or suboptimal least squares (SOLS) routines are used [Billings and Voon 1984] estimates of the process model $G^u[u(t)]$ only are obtained and alternative model validity tests need to be derived.

Estimates of the process model parameters using an IV or SOLS routine will only be unbiased if the noise is additive at the output [Billings and Voon 1984]. These algorithms can therefore only be applied if the model of eqn (6) can be expressed as

$$z(t) = G^u[u(t)] + G^e[e(t)] \tag{8}$$

Model validity tests must be designed therefore to detect the presence of $G^u[u(t)]$ and $G^{ue}[u(t),e(t)]$ terms in the residuals and not $G^e[e(t)]$ since $\xi(t) = G^e[e(t)]$ when no noise model is estimated. If $G^{ue}[u(t),e(t)]$ is detected this will indicate that the noise is not additive at the output and consequently application of IV or SOLS will yield biased estimates. The advantage of considering IV or SOLS algorithms rather than a prediction error routine [Billings and Voon 1985] is that the former two methods involve a considerably reduced parameter set because unbiased estimates can be obtained without fitting a noise model providing the noise is additive at the system output.

The cross-correlation $\phi_{u^{2'}\xi^2}(\tau)$ detects all terms in $G^u[u(t)]$ and $G^{ue}[u(t),e(t)]$ except $G^e[e(t)]$ and is defined as

$$\phi_{u^{2'}\xi^2}(\tau) = E\{[u^2(t)-\overline{u^2(t)}][G^u[u(t+\tau)]+G^{ue}[u(t+\tau),e(t+\tau)]+G^e[e(t+\tau)]]^2\}$$

$$= E\{u^{2'}(t)(G^u[u(t+\tau)])^2+u^{2'}(t)(G^{ue}[u(t+\tau),e(t+\tau)])^2$$

$$+ u^{2'}(t)(G^e[e(t+\tau)])^2\}+2E\{u^{2'}(t)G^u[u(t+\tau)]G^{ue}[u(t+\tau),$$

$$e(t+\tau)]+u^{2'}(t)G^u[u(t+\tau)]G^e[e(t+\tau)]+u^{2'}(t)G^e[e(t+\tau)]$$

$$G^{ue}[u(t+\tau),e(t+\tau)]\} \tag{9}$$

Expanding equation (9) and analysing each term:-

(i) $E\{u^{2'}(t)(G^u[u(t+\tau)])^2\} \neq 0 \;\forall\, G^u[u(t)]$

(ii) $E\{u^{2'}(t)(G^{ue}[u(t+\tau),e(t+\tau)])^2\} \neq 0 \;\forall\, G^{ue}[u(t),e(t)]$

(iii) $E\{u^{2'}(t)(G^e[e(t+\tau)])^2\} = 0 \;\forall\, G^e[e(t)]$

(iv) $E\{u^{2'}(t)G^u[u(t+\tau)]G^{ue}[u(t+\tau),e(t+\tau)]\} = 0$ if for $G^{ue}[u^m e^n]$, n = odd and odd order momentsof $e(t)$ are zero

(v) $E\{u^{2'}(t)G^u[u(t+\tau)]G^e[e(t+\tau)]\} = 0$ if for $G^u[u^m]$ and $G^e[e^n]$, m or n = odd and odd order moments of $e(t)$ and or $u(t)$ are zero

(vi) $E\{u^{2'}(t)G^e[e(t+\tau)]G^{ue}[u(t+\tau),e(t+\tau)]\} = 0$ if $G^{ue}[u^m e^n]$, m = odd and odd order moments of $u(t)$ are zero

Notice that $\phi_{u^{2'}\xi^2}(\tau)$ detects all terms of equation (6) except $G^e[e(t)]$ and therefore $\phi_{u^{2'}\xi^2}(\tau) = 0$ indicates that $G^u[u(t)]$ is correctly modelled and $G^{ue}[u(t),e(t)]$ is zero.

Ideally, it would be desirable if either even or odd polynomial terms could be detected in $G^u[u(t)]$ when $\phi_{u^{2'}\xi^2}(\tau) \neq 0$. This would greatly aid the decision of which polynomial terms should be included in the model. The function $\phi_{u\xi}(\tau)$ detects odd terms in $G^u[u(t)]$ whenever odd moments of u(t) are zero. Conversely $\phi_{u^{2'}\xi}(\tau)$ detects all even terms in $G^u[u(t)]$ (all odd terms make no contribution) again providing the odd order moments of u(t) are zero. Notice however, that both $\phi_{u\xi}(\tau)$ and $\phi_{u^{2'}\xi}(\tau)$ do not indicate the presence of $G^e[e(t)]$ terms in the residuals.

A nonlinear model estimated using IV or SOLS will therefore only be unbiased providing

$$\left.\begin{aligned} &\phi_{u^{2'}\xi^2}(\tau) = 0 \;\forall\tau \\ &\phi_{u^{2'}\xi}(\tau) = 0 \;\forall\tau \\ &\phi_{u\xi}(\tau) = 0 \;\forall\tau \end{aligned}\right\} \tag{10}$$

Sometimes $u^{2'}(t)$ and $\xi^2(t)$ are small and the correlation $\phi_{u^{2'}\xi^2}(\tau)$ may also be small even though $\xi(t)$ is correlated with u(t). It is advisable therefore to include $\phi_{u^{2'}\xi}(\tau)$ and $\phi_{u\xi}(\tau)$ in the model validity checks.

The model validity tests in eqn (10) can indicate which terms have been omitted from the model. An indication of how to interpret the results is summarised in Table 1.

$\phi_{u^{2'}\xi^2}(\tau)$	$\phi_{u^{2'}\xi}(\tau)$	$\phi_{u\xi}(\tau)$	Comment
$= 0$	$= 0$	$= 0$	Process model unbiased. Noise additive at the output
$\neq 0$	$= 0$	$= 0$	Internal noise term $\alpha u^k(t)e^\ell(t)$ where k = even or odd, ℓ odd omitted from the model if odd order moments of $e(t)$ are zero
$\neq 0$	$\neq 0$	$\neq 0$	Internal noise and/or wrong model structure
$\neq 0$	$\neq 0$	$= 0$	Even power of $u(t)$ and/or internal noise $\alpha u^k(t)e^\ell(t)$ k,ℓ = even omitted from the model if odd order moments of $u(t)$ are zero
$\neq 0$	$= 0$	$\neq 0$	Odd power of $u(t)$ and/or internal noise $u^k(t)e^\ell(t)$ k = odd, ℓ = even omitted from the model if odd order moments of $u(t)$ are zero

Table 1

Practical experience in applying the tests developed above has shown that if the tests in both eqn's (7) and (10) are used in conjunction with a prediction error estimation routine this often provides the experimenter with a great deal of information about the system under test and can indicate which terms should be included in the model to improve the fit [Billings and Voon 1985].

Computation Aspects

All the tests above are based on single dimensional correlation functions which for sampled input and output signals are calculated accordingly to the formulae

$$\hat{\phi}_{x'y'}(k) = \frac{\frac{1}{N}\sum_{t=1}^{N-k}(x(t)-\bar{x})(y(t+k)-\bar{y})}{\sqrt{\phi_{x'x'}(0)\phi_{y'y'}(0)}} \tag{11}$$

and similarly $\hat{\phi}_{x'y}(k) = \hat{\phi}_{x'y'}(k)$ with $\bar{y}$ set to zero. The normalisation of the correlation functions as in eqn (11) ensures that they lie in the range

$$-1 \leq \hat{\phi}_{x'y'}(k) \leq 1 \text{ and}$$
$$-1 \leq \hat{\phi}_{x'y}(k) \leq 1.$$

Confidence intervals plotted on the graphs indicate if the correlation between variables is significant or not. If N is large the standard deviation of the correlation estimate is $1/\sqrt{N}$, the 95% confidence limits are therefore approximately $\pm 1.96/\sqrt{N}$.

Simulation Results

The algorithms described above have been tested on both simulated systems and industrial plant data.

An implicit nonlinear model was simulated with additive coloured noise

$$y(t) = 0.5y(t-1) + 0.3y(t-1)u(t-1) + 0.2u(t-1) + 0.6u^2(t-1) + 0.05y^2(t-1) \tag{12}$$

$$z(t) = y(t) + e(t) + 1.5e^2(t) + 0.5e^3(t)$$

$u(t) = u'(t)+b$, $b = 0.2$ and $e(t)$ a discrete white sequence $\mathcal{N}(0,0.1)$.

The mean levels of equation (12), $\overline{z_b} = 0.1623$ and $\bar{z} = 1.249$ indicate that the process is nonlinear and this is confirmed by $\phi_{z'z'^2}(\tau)$ and $\phi_{z_b'z_b'^2}(\tau)$ in figure 1.

A suboptimal least squares algorithm was used to estimate the parameters in equation (12). To illustrate the effectiveness of the model validity tests derived for this type of system the term $0.3y(t-1)u(t-1)$ was deliberately omitted from the model and the parameters were estimated using suboptimal least squares to yield the model

$$z(t) = 0.05975z(t-1) + 0.3303u(t-1) + 0.1213z^2(t-1) + 1.198u^2(t-1) \tag{13}$$

The correlation functions $\phi_{u\xi}(\tau)$, $\phi_{u^{2'}\xi}(\tau)$ and $\phi_{u^{2'}\xi^2}(\tau)$ in figure 2 indicate that the model (equation 13) is biased. However including all the terms in the model yields final estimates as

$$z(t) = 0.5135z(t-1) + 0.1932u(t-1) + 0.04377z^2(t-1) + 0.3113z(t-1)u(t-1) + 0.5969u^2(t-1) \tag{14}$$

The model validity tests indicate that this model is adequate as illustrated in figure 3 and shown by comparison of equation (12) and (14).

A heat exchanger consisting of a radiator through which heated water is passed and a fan which blows air across the radiator was studied [Billings and Fadzil 1985]. The system is a two input (heater and fan controls), two output (drop in temperature across the radiator, air flow rate) system. Models have been fitted to all the loops only one of which is nonlinear. Only the nonlinear fan/air flow loop will be considered here. Initially a linear model was estimated using a prediction error routine to yield the best linear model

$$\begin{aligned} z'(t) = {} & 0.851z'(t-1) - 0.1571z'(t-2) \\ & + 0.265u'(t-1) - 0.333u'(t-2) + \varepsilon(t) \\ & - 0.0894\varepsilon(t-1) + 0.339\varepsilon(t-2) + 0.227\varepsilon(t-3) \\ & + 0.0813\varepsilon(t-4) \end{aligned} \qquad (15)$$

Computing the residuals for this model and applying the model validity tests of both eqns (7) and (10) gave the results illustrated in Fig.4. Because $\phi_{\xi\xi}(\tau) = \delta(\tau)$ and $\phi_{u\xi}(\tau) = 0 \ \forall\tau$ in Fig.4 a normal linear analysis would terminate at this point, and the poor prediction accuracy of the model would probably be assumed to be caused by a poor S/N ratio. Inspection of Fig.4 however clearly shows that $\phi_{u^{2'}\xi}(\tau)$ and $\phi_{u^{2'}\xi^2}(\tau)$ are well outside the 95% confidence bands indicating that nonlinear terms should be included in the model. The input excitation for the heat exchanger was a Gaussian white signal so that from Table 1, the combination of $\phi_{u\xi}(\tau) = 0$, $\phi_{u^{2'}\xi}(\tau) \neq 0$ and $\phi_{u^{2'}\xi^2}(\tau) \neq 0$ strongly suggests that even terms (e.g. $u^2(\cdot)$) and/or internal noise terms of the form $u^k(t)\varepsilon^\ell(t)$ ℓ,k even should be added to the model. Since $\phi_{\xi\xi u}(\tau)$ is within the confidence bands this indicates that there are no terms of the form $u^q(t-m)\varepsilon(t-n) \ \forall \ n,m$, odd q in the residuals. The effects of introducing these nonlinear terms in the model was therefore investigated.

A prediction error estimator combined with a stepwise regression algorithm was used to determine which nonlinear terms to include in the model and to optimise the parameter estimates. The use of this algorithm in combination with the model validity tests of eqns (7) and

(10) produced the final nonlinear model [Billings and Fadzil 1985]

$$\begin{aligned} z(t) = {} & 2.301+0.9173z(t-1)+0.449u(t-1)+0.04577u(t-2) \\ & -0.01889z^2(t-1)-0.00999u^2(k-1)-0.002099z^2(t-1)u(t-1) \\ & -0.00243u^3(t-1)+\varepsilon(t)-0.004\varepsilon(t-1)+0.038\varepsilon(t-2) \\ & +0.2745\varepsilon(t-3)+0.1037\varepsilon(t-4) \end{aligned} \tag{16}$$

The structure of eqn (16) was obtained by combining the information from the stepwise regression/prediction error algorithm with the results of the model validity tests eqn's (7), (10) in an iterative manner. Full details are given elsewhere. The model validity tests for the model of eqn (16) which are illustrated in Fig.5 are all within the confidence bands indicating that the residuals are unpredictable from all linear and nonlinear combinations of past inputs and outputs.

Conclusions

Model validity tests for nonlinear systems have been developed. It has been shown that the traditional covariance tests developed for linear systems provide incorrect information when applied to nonlinear systems and new tests based on higher order correlation functions have been derived. The application and interpretation of these tests to both simulated and real data has been demonstrated.

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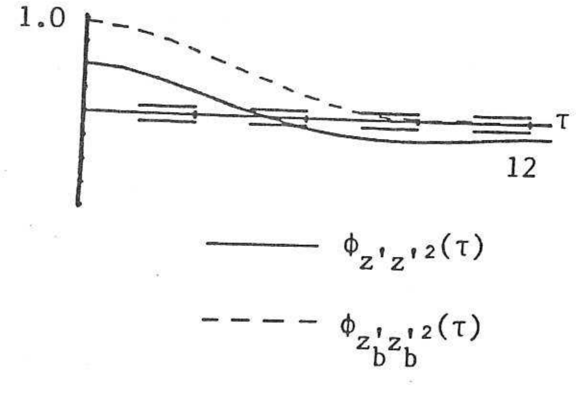

Fig.1. Testing for nonlinearity

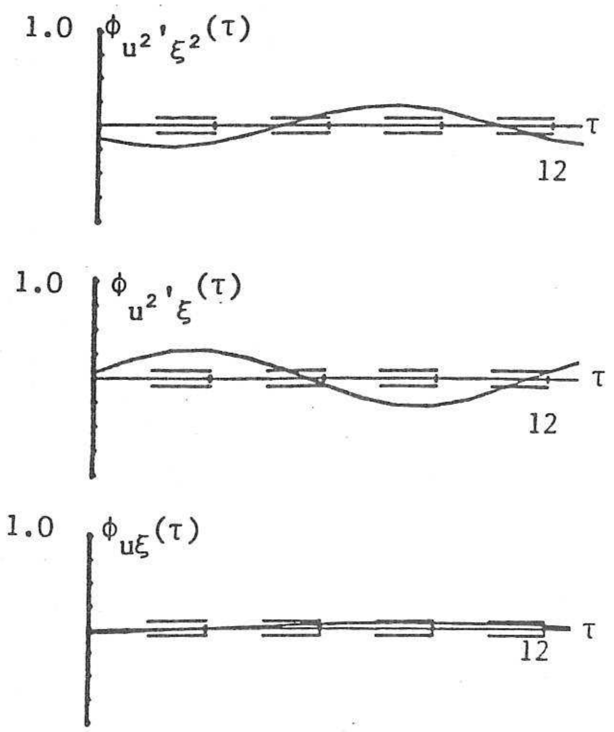

Fig.2. Model Validation

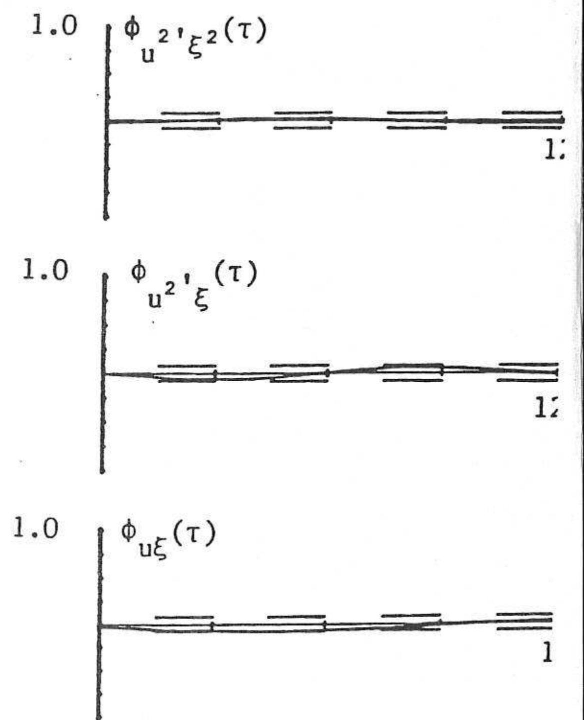

Fig.3. Model Validation

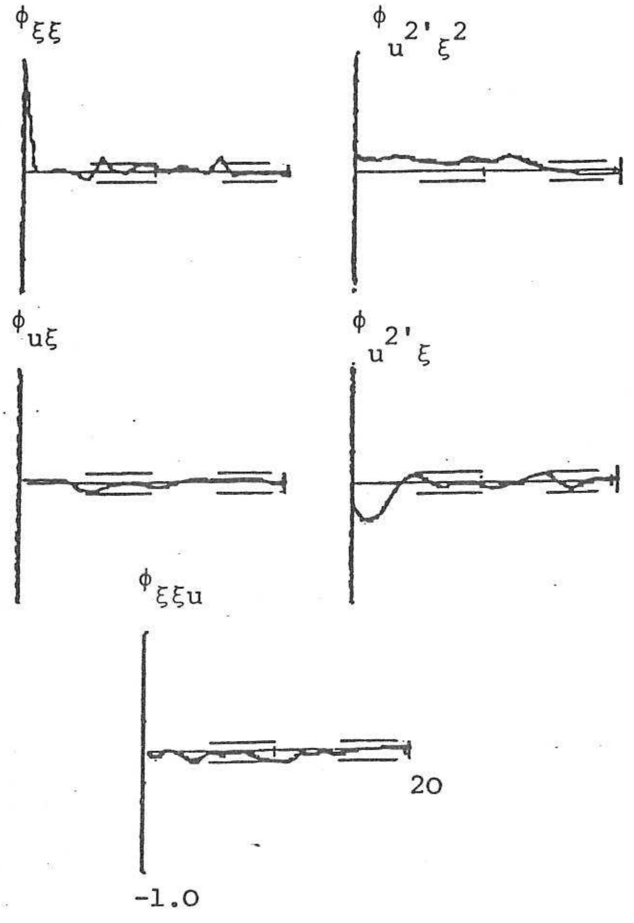

Fig.4. Validity tests - best linear model

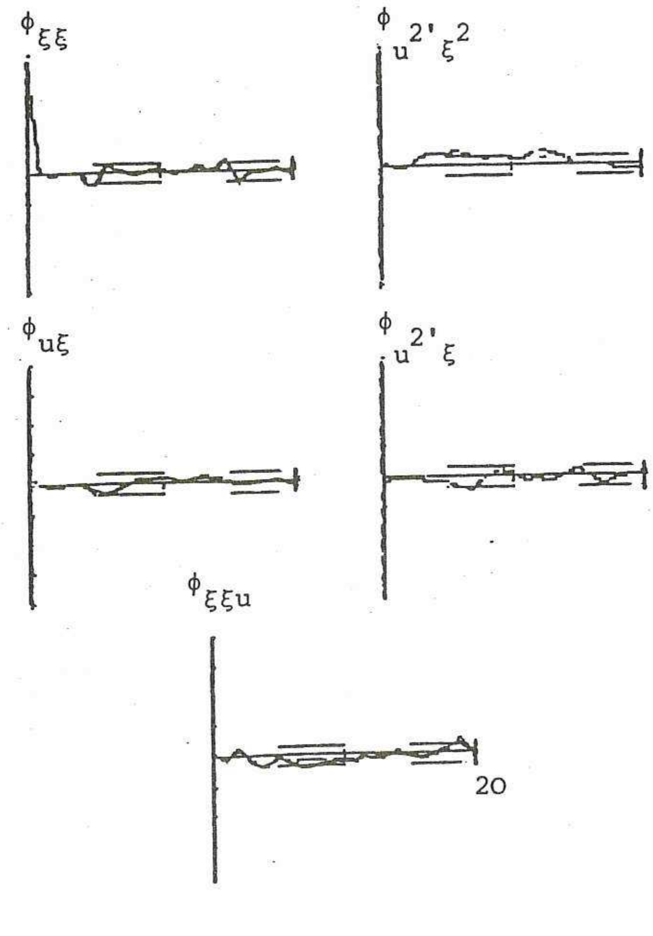

Fig.5. Validity tests - best nonlinear model