Forward-backward kernel-based state and parameter estimation for linear systems of arbitrary order

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Abstract

Previous results pertaining to algebraic state and parameter estimation of linear systems based on a special construction of a forward-backward kernel representation of linear differential invariants are extended to handle large noise in output measurement. Explicit expressions for the kernel functions for single-input, single-output (SISO) linear time-invariant (LTI) systems of arbitrary order are first stated and proved. A two-stage solution of the estimation problem is proposed next. The parameter estimation sub-problem, which is the task of the first stage, is solved by way of stochastic regression. The parameter estimation method presented in earlier publications is enhanced using multiple regression. The regression model does not satisfy the assumptions of the Gauss-Markov theorem in that the random regressor is heteroskedastic. This does not impede achieving high accuracy of estimation. A recursive version of a feasible generalized least squares with covariance weighting is employed to attenuate adverse effects due to heteroskedasticity. The output of the system and its time derivatives are reconstructed smoothly in the second stage of the approach by way of projection, while minimizing a mean square criterion.
1 Introduction

The body of work on system identification and filtering is extremely vast; to cite merely a few leading texts in the area, [1], [2], [3], [4]. Recursive approaches prevail, primarily rooted in Kalman’s seminal work, [5], justified by computational efficiency with limited data delivered sequentially.

In contrast, the problem considered here is related to joint parameter and state estimation but over a finite interval of time whose length is only constrained by the requirement of identifiability of the system from a single realization of stochastic measurement process, but with no restriction on the quantity of measured samples. The interest in such a problem is perhaps best explained by the following application. Consider a noisy measurement signal as shown in Figure 1 which is stipulated to obscure a smooth trajectory of a dynamical object. Is it possible to predict the motion of the object, without error, far beyond the observation interval? A positive answer is conditioned on the ability to retrieve a deterministic ‘law of motion’ for the object from the noisy data. One such ‘law of motion’ is a differential invariant of the system, i.e. an expression binding the output variable and its derivatives that remain constant under the action of the system flow. As the differential invariant persists, the trajectory of the system can be extrapolated as desired.

Needless to remark that, as first appreciated in the seminal work of [6], the above problem has other countless applications, all of which call for highest estimation precision in shortest possible time, often in the presence of high levels of measurement noise of unknown characteristics. To mention only a few: the need for non-asymptotic estimation methods as justified by modern developments in systems with rapidly switching dynamics, [7], advanced nonlinear control design based on differential flatness, [8], and the demand for powerful target tracking algorithms of superior performance in speed and precision, [9]. The issue of handling extreme measurement noise becomes especially relevant in the case of applications in astronomy.

The idea of constructing kernel representations of differential invariants, as first presented in [10], and continued in [11], [12], [13], [14], [15], [16], initially sprung from an attempt to improve on the algebraic signal differentiation approach proposed in [17], [18], as the principal tool required in the implementation of controllers for nonlinear systems that are differentially flat. The original algebraic differentiator was based on truncated Taylor series signal approximation and attributed its properties to the introduction of an algebraic annihilator of the Taylor series coefficients up to any desired order; see [17], [19], [20], and [21]. After iterated integration it then delivered the values of the selected coefficients that escaped annihilation, effectively the values of the desired higher order derivatives. The annihilator served yet a different purpose: that of shaping the noise rejection characteristic of the resulting ‘filter’; see [22]. As was admitted, however, the method required frequent re-initialization when used forward in time, and its noise rejection properties were characterized as non-standard; see [23]. In spite of the power of non-standard analysis methods, [24], used in [23] as well as the efforts to attenuate measurement noise by designing
SNR-maximizing annihilators and pre-filters, it was still admitted in [18] that algebraic estimation is very sensitive to noise. It thus became clear, that any further improvements hinged on the application of more rigorous statistical and probabilistic framework.

With the above introduction the contributions made here are summarized as follows:

• Although the double sided kernel representation of both free and controlled system invariance has been used in a series of brief contributions, [10], [11], [12], [13], [15], the explicit expressions for the kernel representation of linear differential invariants of arbitrary order are delivered here; their validity is supported by proofs and implications are listed.

It is worth noting that there are methods reported in the literature; see [25], [26], [2], for identification of finite-impulse responses of stable LTI systems based on the use of Gaussian kernels, which are powerful tools in stochastic estimation and machine learning. Special mention must also be made of the Rauch-Tung-Striebel smoother which works in conjunction with the Kalman filter over a fixed interval, [27], [28], [29], [30]; see Section 7.1 for a comparison. Yet another approach is presented in [31] in the way of functional data analysis. However, the kernels presented here have the unique advantage of being ‘tailored’ specifically to capture the deterministic counterpart of a ‘covariance structure’ behind the dynamical trends imposed by the class of linear differential invariance models. More precisely, the double-sided kernels are parametrized by the coefficients in the invariance functions and are in fact exact interpolating splines for trajectories generated by invariants with matching coefficients (the double-sided kernels are somewhat similar to L-splines; see [32]). Another useful attribute of the kernels introduced here is that they contain two-sided annihilators of any boundary conditions, which can be shaped towards improved noise attenuation; a possibility not needed here.

• Additionally, the constructed kernels naturally induce a reproducing kernel Hilbert space in which invariance orbits can be reconstructed using the RKHS kernel basis without the adverse effects of overfitting hence rendering regularization redundant. By virtue of the represented theorem in the induced RKHS the derivatives of the invariance orbits of any order can then be calculated as integral transforms of the reconstructed orbit itself; see [33]. Finally, in contrast to the Taylor series based estimation and differentiation methods of [34], [17], [19], and [20], the proposed double-sided kernels do not exhibit any singularities at the extremities of the estimation interval and eliminate the need for re-initialization to compensate for accumulation of numerical errors.

• To demonstrate the power of invariance in the role of a deterministic backbone of kernel-based estimation, a fourth order SISO LTI homogeneous unstable system is considered, in which the invariance originates from its characteristic equation. A homogeneous system is chosen for the purpose of a more interesting demonstration as closed-loop systems are more difficult to identify because there is no input to deliver persistent excitation; see [2]. The objective is to estimate the parameters and reconstruct the invariance orbit together with its three derivatives from a single realization of a measurement process with large
additive Gaussian noise whose variance is unknown. The resulting stochastic regression model, however, fails to satisfy the assumptions of the Gauss-Markov Theorem calling for the use of approaches that can secure consistency and eliminate the effects of heteroskedasticity. This problem is addressed by employing standard remedies such as a recursive version of the feasible generalized least squares with covariance weighting, [35], [36]. A criterion for practical identifiability is introduced and stochastic aspects of orbit and derivative reconstruction are discussed.

- The feasible recursive least squares algorithm for parameter estimation is further improved by using multiple regression equations. Using the reproducing property of kernels, the kernels are integrated multiple times forming multiple linearly independent regression equations — so that the number of regression equations in total matches the number of unknown parameters. The covariance weighting scheme is modified accordingly to tackle heteroskedasticity. This approach yields results comparable to those in [16] — but here similar performance is achieved with considerably reduced number of samples.

The paper is structured as follows. The finite interval estimation problem is stated in Section 2. Section 3 delivers the kernel representation of linear differential invariance. Parametric estimation of the differential invariance is stated as a least squares problem in Section 4. Identifiability of closed loop LTI systems from a single output trajectory is briefly discussed followed by comments about the properties of the regression problem formulation that leads to the introduction of a method to compensate for heteroskedasticity. Parametric estimation using multiple regression is discussed in Section 5. Error covariance matrices are computed for the modified covariance weighting scheme to tackle heteroskedasticity. Section 6 describes the simplest method to reconstruct the output trajectory and its derivatives. Section 7 presents simulation results and their discussion, along with a comparison with the Unscented Rauch-Tung-Striebel smoother. Section 8 delivers the conclusion and is followed by References. Appendices A-B contain the proofs of the representation theorems. Appendix C gives the expressions for 4th order kernels. Appendix D states the details of the feasible recursive GLS algorithm and its initialization.

2 A finite interval estimation problem for an LTI system

Consider a general $n$-th order, strictly proper and minimal SISO LTI system in state space form evolving on a given finite time interval $[a, b] \subset \mathbb{R}$:

$$\begin{align*}
\dot{x} &= Ax + bu ; \\
y &= c^T x ; \\
x &\in \mathbb{R}^n
\end{align*}$$

with matching dimensions of the system matrices and the characteristic equation

$$\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_1\lambda + a_0 = 0$$

4
The input-output equation for system (1) becomes
\[ y^{(n)}(t) + a_{n-1}y^{(n-1)}(t) + \cdots + a_1y^{(1)}(t) + a_0y(t) = -b_{n-1}u^{(n-1)}(t) - \cdots - b_0u(t) \] (3)

where \(-b_i, i = 0, \ldots, n-1\) are the coefficients of the polynomial in the numerator of the rational transfer function for (1).

The estimation problem is stated as follows. Given an arbitrary finite interval of time \([a, b]\), suppose that:

(i) The dimension of the state vector of the LTI system is known a priori alongside the system input function \(u(t)\) with its derivatives \(u^{(i)}(t), i = 1, \cdots, n-1\) for \(t \in [a, b]\) (implicit is the statement that the \(u\) is \(n-1\) times differentiable);

(ii) The output of the system is observed as a single realization of a ‘continuous’ measurement process \(y_M(t) := y(t) + \eta(t), t \in [a, b]\) in which \(\eta\) denotes additive white Gaussian noise with unknown intensity (variance) \(\sigma^2\).

Although some of the derivations in this paper will indeed employ continuous representation of the measurement process, an implementable version of assumption (ii) simply requires availability of an unrestricted number of output measurements over the observation horizon \([a, b]\).

Under these conditions it is required that:

(a) Identifiability of the system input-output parameters \(a_i, b_i, i = 0, \cdots, n-1\) from a single realization of the measurement process \(y_M(t), t \in [a, b]\) be determined for the given observation horizon \([a, b]\);

(b) Under identifiability condition, a parameter estimator for \(a_i, b_i, i = 0, ..., n-1\) be proposed that is statistically consistent;

(c) The true system output \(y(t)\) and its \(n-1\) time derivatives \(y^{(i)}(t), i = 1, \ldots, n-1\) be reconstructed from the noisy observation \(y_M(t)\) over \(t \in [a, b]\);

(d) The reconstruction error in the output function \(y\) and its derivatives \(y^{(i)}, i = 1, \ldots, n-1\) converges to zero uniformly as the number of measurement samples of \(y_M\) increases freely.

It is worth pointing out that assumption (i) requesting complete knowledge of the system input and its derivatives is not absolutely necessary. The approach can be potentially extended to the case when the input function is also identified using B-splines or other non-parametric representations.

For simplicity of exposition, the estimation approach is presented here with respect to the more interesting case of homogeneous systems in which persistent excitation cannot be rendered by way of the system input \(u\). Without the loss of generality, the order of the system considered in an example demonstration of the validity and properties of the approach is taken to be \(n = 4\).
3 A kernel representation of a system differential invariance

The cornerstone of the finite interval estimation approach presented here is the integral representation of the controlled differential invariance of the system (3). For the homogeneous system the latter is given by a mapping

$$J(y, y^{(1)}, \ldots, y^{(n)}) := y^{(n)}(t) + a_{n-1}y^{(n-1)}(t) + \cdots + a_1y^{(1)}(t) + a_0y(t)$$

$$\equiv \text{const.} = 0; \quad t \in [a, b]$$ (4)

that remains constant under the action of the flow of the system in the absence of external forcing. The validity of (4) is seen to deliver additional measurement-noise independent information about the behaviour of the system beyond mere observation of the noisy $y_M$. To be useful, however, the 'zero-input response' characterization (4) has to be put in a form, which does not depend on the initial or boundary conditions of the system, and that does not involve any time derivatives of the output as the last are not available through direct measurement. Such a system characterization is given in terms of the Theorems below, but is preceded by a helpful definition.

**Definition 1** A pair of smooth (class $C^\infty$) functions $(\alpha_a, \alpha_b)$, $\alpha_s : [a, b] \to \mathbb{R}$, $s = a$ or $b$, is an annihilator of the boundary conditions for system (1) if the functions $\alpha_s$ are non-negative, monotonic, vanish with their derivatives up to order $n-1$ at the respective ends of the interval $[a, b]$; i.e.

$$\alpha_s^{(i)}(s) = 0; \quad i = 0, \ldots, n-1; \quad s = a, b; \quad \alpha_s^{(0)} \equiv \alpha_s$$

and such that their sum is strictly positive, i.e. that for some constant $c > 0$

$$\alpha_{ab}(t) := \alpha_a(t) + \alpha_b(t) > c; \quad t \in [a, b]$$ (6)

A simplest example of such an annihilator for (1) is the pair

$$\alpha_a(t) := (t-a)^n, \quad \alpha_b(t) := (b-t)^n; \quad t \in [a, b]$$

$$\alpha_{ab}(s) = (b-a)^n, \quad s = a, b$$ (7)

Indeed, it is easy to see that (7) holds for all $n \geq 1$ because $\alpha_{ab}(a) = \alpha_{ab}(b) = (b-a)^n > 0$ and, for $n \geq 2$, $\alpha_{ab}$ has a unique stationary point $t^* = 0.5(a+b) \in [a, b]$ at which $\alpha_{ab}(t^*) = (0.5)^{n-1}(b-a)^n$.

Employing this particular annihilator, an integral representation for system (1) is rendered by the following:
Theorem 1 There exist Hilbert-Schmidt kernels $K_{DS,y}, K_{DS,u}$, such that the input and output functions $u$ and $y$ of (1) satisfy

$$y(t) = \alpha_{ab}^{-1}(t) \left[ \int_a^b K_{DS,y}(n,t,\tau)y(\tau)d\tau + \int_a^b K_{DS,u}(n,t,\tau)u(\tau)d\tau \right]$$

with

$$\alpha_{ab}^{-1}(t) := \frac{1}{(t-a)^n + (b-t)^n}$$

Hilbert-Schmidt double-sided kernels of (8) are square integrable functions on $L^2[a,b] \times L^2[a,b]$ and are expressed in terms of the ‘forward’ and ‘backward’ kernels given below:

$$K_{DS,y}(n,t,\tau) \triangleq \begin{cases} K_{F,y}(n,t,\tau), & \text{for } \tau \leq t \\ K_{B,y}(n,t,\tau), & \text{for } \tau > t \end{cases}$$

$$K_{DS,u}(n,t,\tau) \triangleq \begin{cases} K_{F,u}(n,t,\tau), & \text{for } \tau \leq t \\ K_{B,u}(n,t,\tau), & \text{for } \tau > t \end{cases}$$

The kernel functions $K_{DS,y}, K_{DS,u}$ are $n-1$ times differentiable as functions of $t$.

The forward and backward kernels of (10) have the following expressions:

$$K_{F,y}(n,t,\tau) = \sum_{j=1}^{n} (-1)^{j+1} \binom{n}{j} \frac{n!(t-\tau)^{j-1}(\tau-a)^{n-j}}{(n-j)!(j-1)!}$$

$$+ \sum_{i=0}^{n-1} a_i \sum_{j=0}^{i} (-1)^{j+1} \binom{i}{j} \frac{n!(t-\tau)^{n-i+j-1}(\tau-a)^{n-j}}{(n-j)!(n-i+j-1)!}$$

$$K_{B,y}(n,t,\tau) = \sum_{j=1}^{n} \binom{n}{j} \frac{n!(t-\tau)^{j-1}(b-\tau)^{n-j}}{(n-j)!(j-1)!}$$

$$+ \sum_{i=0}^{n-1} a_i \sum_{j=0}^{i} \binom{i}{j} \frac{n!(t-\tau)^{n-i+j-1}(b-\tau)^{n-j}}{(n-j)!(n-i+j-1)!}$$

$$K_{F,u}(n,t,\tau) = \sum_{i=0}^{n-1} b_i \sum_{j=0}^{i} (-1)^{j+1} \binom{i}{j} \frac{n!(t-\tau)^{n-i+j-1}(\tau-a)^{n-j}}{(n-j)!(n-i+j-1)!}$$

$$K_{B,u}(n,t,\tau) = \sum_{i=0}^{n-1} b_i \sum_{j=0}^{i} \binom{i}{j} \frac{n!(t-\tau)^{n-i+j-1}(b-\tau)^{n-j}}{(n-j)!(n-i+j-1)!}$$

The proof is found in Appendix A and is essentially conducted by construction, involving the induction argument only at its final stage. Therefore, the
only loss of information in the passage from the input-output equation of the system to the integral kernel representation in Theorem 1 is that of any preexisting boundary conditions in (3) as the latter are annihilated during every integration operation by the presence of the annihilating factors $\alpha_a$ and $\alpha_b$. The following conjecture is then quite obvious.

**Corollary 1** For any given input function $u$, the output function $y : [a, b] \rightarrow \mathbb{R}$ satisfies the system input-output equation (3) on the interval $[a, b]$ if and only if it satisfies the integral equation (8) regardless of any boundary conditions that may be imposed. The kernel representation of the system invariance provides a unique criterion whose reproducing property unambiguously characterizes all zero input solutions of the SISO LTI system. In particular all the fundamental solutions of the LTI system share the reproducing property (8) as they span a subspace of the RKHS of dimension $n$.

\[ \square \]

**Explicit kernel expressions for the derivatives of the output function:**

Due to the regularity properties of the kernel functions in Theorem 1, it is straightforward to obtain the corresponding recursive formulae for the time derivatives of the system output, $y^{(i)}$, $i = 1, \cdots, n - 1$.

**Theorem 2** There exist Hilbert-Schmidt kernels $K_{F,k,y}$, $K_{F,k,u}$, $K_{B,k,y}$, $K_{B,k,u}$, $k = 1, \cdots, n - 1$ such that the derivatives of the output function in (1) can be computed recursively as follows:

\[
y^{(k)}(t) = \frac{1}{(t-a)^n + (b-t)^n} \left[ \sum_{i=1}^{k} (-1)^{i+1} \binom{p+i-1}{i} \frac{n!(t-a)^{n-i}y^{(k-i)}(t)}{(n-i)!} \\
+ \sum_{i=p}^{n-1} a_i \sum_{j=0}^{i-p} (-1)^{j+1} \binom{p+j-1}{j} \frac{n!(t-a)^{n-j}y^{(i-j-p)}(t)}{(n-j)!} \\
+ \int_{a}^{t} K_{F,k,y}(n,p,t,\tau)y(\tau)d\tau + \int_{a}^{t} K_{F,k,u}(n,p,t,\tau)u(\tau)d\tau \\
+ \sum_{i=p}^{n-1} b_i \sum_{j=0}^{i-p} (-1)^{j+1} \binom{p+j-1}{j} \frac{n!(b-t)^{n-j}y^{(i-j-p)}(t)}{(n-j)!} \\
- \sum_{i=1}^{k} \binom{p+i-1}{i} \frac{n!(b-t)^{n-i}y^{(k-i)}(t)}{(n-i)!} \\
+ \sum_{i=p}^{n-1} a_i \sum_{j=0}^{i-p} (-1)^{j+1} \binom{p+j-1}{j} \frac{n!(b-t)^{n-j}y^{(i-j-p)}(t)}{(n-j)!} \\
+ \int_{t}^{b} K_{B,k,y}(n,p,t,\tau)y(\tau)d\tau + \int_{t}^{b} K_{B,k,u}(n,p,t,\tau)u(\tau)d\tau \right]
\]
where $p = n - k$ and

$$
K_{F,k,y}(n,p,t,\tau) = \sum_{j=1}^{p} (-1)^{j+n-p+1} \binom{n}{n-p+j} \frac{n!(t-\tau)^{j-1}(\tau-a)^{p-j}}{(p-j)! (j-1)!} \\
+ \sum_{i=0}^{p-1} a_i \sum_{j=1}^{n} (-1)^{i+j} \binom{j}{i} \frac{n!(t-\tau)^{i+j-1}(\tau-a)^{n-j}}{(n-j)! (p-i+j-1)!} \\
+ \sum_{i=p}^{n-1} a_i \sum_{j=1}^{p} (-1)^{i+j-p+1} \binom{i}{i-p+j} \frac{n!(t-\tau)^{i-j-1}(\tau-a)^{n-i+p-j}}{(n-i+p-j)! (j-1)!}
$$

$$
K_{B,k,y}(n,p,t,\tau) = \sum_{j=1}^{p} \binom{n}{n-p+j} \frac{n!(t-\tau)^{j-1}(b-\tau)^{p-j}}{(p-j)! (j-1)!} \\
+ \sum_{i=0}^{p-1} a_i \sum_{j=1}^{n} \binom{j}{i} \frac{n!(t-\tau)^{p-i+j-1}(b-\tau)^{n-j}}{(n-j)! (p-i+j-1)!} \\
+ \sum_{i=p}^{n-1} a_i \sum_{j=1}^{p} \binom{i}{i-p+j} \frac{n!(t-\tau)^{i-j-1}(b-\tau)^{n-i+p-j}}{(n-i+p-j)! (j-1)!}
$$

**Remark 1.** It is important to note that for $u \equiv 0$, the invariance representation [8] is in fact a continuous evaluation functional for the system output functions and hence induces a unique reproducing kernel Hilbert space (RKHS) with kernel

$$
K_y(t_1,t_2) := \alpha_{ab}^{-2}(t) \int_{a}^{b} K_{DS,y}(t_1,\tau) K_{DS,y}(t_2,\tau) d\tau \quad (11)
$$

$t_1, t_2 \in [a,b]$ where the dependence of the kernels on the system order $n$ has been suppressed for brevity; see [37] for more details. The kernel (11) can in
fact be regarded as a deterministic counterpart of a ‘covariance structure’ of a process whose trend is described in terms of the differential invariant. It then also follows that any bounded linear functional \( L : y \to L(y)(t) \) on the RKHS space has a representer, which is the kernel \( L(K_y(t, \cdot)) \). This kernel trick and other properties of the RKHS have vast implications for estimation in RKHS, see [38], [39], followed by [40]. The properties of the kernels established by Theorem 1 also imply that approximation of functions in the induced RKHS (such as those needed in output signal reconstruction) can be carried out in some countable basis of ‘feature splines’:

\[
\text{span}\{K_{DS,y}(t_i, \cdot); \ t_i \in [a, b], i \in \mathbb{I}\}
\]  

The expressions for the kernels of Theorem 1 for a 4th order homogeneous LTI system are found in Appendix C.

Given the kernel representation of the system differential invariance, the estimation problem will be solved in two separate stages: (a) parametric estimation of the coefficients of the characteristic equation \( a_i, i = 0, \ldots, n - 1 \); (b) non-parametric estimation/reconstruction of the system output trajectory and its time derivatives over the interval \([a, b]\).

4 Parametric estimation as a least squares problem

As the kernels of Theorem 1 are linear in the unknown system coefficients, the reproducing property (for homogenous systems) is first re-written to bring out this fact while omitting the obvious dependence of the kernels on \( n \) [15]. The term \( \alpha_{ab}(t) \) is subsumed in \( K_{DS} \) for convenience of notation.

\[
y(t) = \int_a^b K_{DS,y}(t, \tau)y(\tau) \, d\tau \tag{13}
\]

\[
= \sum_{i=0}^n \beta_i \int_a^b K_{DS(i),y}(t, \tau)y(\tau) \, d\tau \tag{14}
\]

where the \( K_{DS(i),y}; i = 0, \ldots, n \) are ‘component kernels’ of \( K_{DS,y} \) that post-multiply the coefficients \( \beta_i = a_i; i = 0, \ldots, n \), with \( \beta_n = a_n = 1 \) for convenience of notation. In a noise-free deterministic setting, the output variable \( y \) becomes the measured output coinciding with the nominal output trajectory \( y_T \), so the regression equation for the constant parameters \( a_i, i = 0, \ldots, n - 1 \), [14], can be written in a partitioned form as

\[
y_T(t) = [K^{\bar{a}}, K^{a_n}](t; y_T) \beta \tag{15}
\]

\[
\bar{a} := [a_0; \ldots; a_{n-1}]; \quad \beta := [\bar{a}; 1]
\]

where \( K^{\bar{a}}(t; y_T) \) is a row vector with integral components

\[
K^{\bar{a}}(t; y_T)_k := \int_a^b K_{DS(k),y}(t, \tau)y_T(\tau) \, d\tau \ ; \ k = 0, \ldots n - 1 \tag{16}
\]
while $K^{a_n}(t; y_T)$ is a scalar

$$K^{a_n}(t; y_T) := \int_a^b K_{DS(n),y}(t, \tau) y_T(\tau) d\tau$$

(17)

corresponding to $a_n = 1$.

Given distinct time instants $t_1, \cdots, t_N \in (a, b]$, here referred to as knots, the regression equation is re-written point-wise in the form of a matrix equation

$$Q(y_T) = P(y_T) \bar{a}$$

(18)

$$Q := \begin{bmatrix} q(t_1) \\ \vdots \\ q(t_N) \end{bmatrix}; P := \begin{bmatrix} p_0(t_1) \cdots p_{n-1}(t_1) \\ \vdots \\ p_0(t_N) \cdots p_{n-1}(t_N) \end{bmatrix}$$

$$q(t_i) = y_T(t_i) - K^{a_n}(t_i, y_T); p_k(t_i) = \bar{K}^{a_n}(t_i; y_T)_k$$

(19)

that can be solved using least squares error minimization provided adequate identifiability assumptions are met and the output is measured without error.

**Identifiability of homogeneous LTI systems from a single realization of a measured output:**

Identifiability of homogeneous LTI system such as

$$\dot{x}(t) = Ax(t); \quad y = Cx; \quad x \in \mathbb{R}^n$$

$$x(0) = b$$

(20)

from a single noise-free realization of its output trajectory $y$ on the interval $[0, \infty)$ has been studied by [41]. The identifiability condition is cited here in an equivalent form as:

**Definition:** System (20) is globally identifiable from $b$ if and only if the functional mapping $A \mapsto y(\cdot; A, b)$ is injective on $\mathbb{R}^n$ where $b$ is fixed and $y(\cdot; A, b)$ denotes the output orbit of (20) through $b$.

The identifiability condition is then rendered by:

**Theorem:** [41] System (20) is globally identifiable from $b$ if and only if the evolution of the output orbit of (20) is not confined to a proper subspace of $\mathbb{R}^n$.

The above criterion has limited use for reasons of practicality: it is difficult to verify computationally, pertains to infinite time horizons $[0, \infty)$ and, most importantly, requires the output trajectory to be known exactly. For the purpose of the present exposition it hence suffices to invoke a practical version of identifiability as defined below.

**Definition 2 (Practical linear identifiability)** The homogeneous system (3) is practically linearly identifiable on $[a, b]$ with respect to a particular noisy discrete realization of the output measurement process, $y_M(t), t \in [a, b]$, if and only if there exist distinct knots $t_1, \cdots, t_N \in (a, b]$ which render $\text{rank} P(y_M) = n$. Any such output realization is then called persistent.
In the presence of measurement noise, here assumed to be AWGN — white Gaussian and additive, the regression equation (14) is no longer valid as the reproducing property fails to hold along an inexact output trajectory. It must thus be suitably replaced leading to a stochastic regression problem. First, the stochastic output measurement process on a suitable space such as $L^2(\Omega, \mathcal{F}, \mathbb{P})$, where $y_M$ is assumed to be adapted to the natural filtration of the standard Wiener process $W$ on $[a, b]$, is

$$y_M(t, \omega) = y_T(t) + \sigma \dot{W}(t, \omega) ; \quad t \in [a, b]$$

where $y_T$ is the true system output and $\dot{W}$ signifies the generalized derivative of the standard Wiener process; see e.g. [42], i.e. $\sigma \dot{W}$ is identified with the white noise process with constant variance $\sigma^2$.

The following facts are standard and are recalled here for later reference; see [42]. The generalized derivative $\dot{W}$ of the Wiener process $W$ is defined by the following equality that needs to hold for all smooth functions $g$ with compact support

$$g(t)W(t) = \int_a^t g(s)\dot{W}(s)ds + \int_a^t \dot{g}(s)W(s)ds ; \quad t \in [a, b]$$

where the argument $\omega$ is omitted for brevity of notation. The integral is well defined

$$\int_a^t g(s)\dot{W}(s)ds, \quad t \in [a, b]$$

for any square integrable function $g$; i.e. $g$ does not have to be smooth, but

$$\int_a^b g^2(s)ds < \infty$$

The generalized expectation and covariance functions of white noise are given by:

$$\mathbb{E}[\dot{W}(t)] = 0$$
$$\text{Cov}[\dot{W}(t)\dot{W}(s)] = \mathbb{E}[\dot{W}(t)\dot{W}(s)] = \delta(t-s)$$
$$\text{Var}[\dot{W}(t)] = \mathbb{E}\left(\dot{W}(t)^2\right) = 1 \quad t, s \in [a, b]$$

where $\delta$ is the delta Dirac distribution (strictly: a linear functional defined on the space of tempered distributions) but acting on square integrable functions as an evaluation functional:

$$\int_a^b g(s)\delta(t-s)ds = g(t), \quad t \in [a, b]$$
Moreover, for any square integrable function \( g \)
\[
E \int_a^t g(s)\dot{W}(s)ds = 0,
\]
\[
E \left( \int_a^t g(s)\dot{W}(s)ds \right)^2 = \int_a^t g^2(s)ds, \quad t \in [a, b]
\] (29)

Now, without adhering to any particular realization of the measurement process \([21]\), the kernel expression
\[
\int_a^b K_{DS,y}(t, \tau) y_M(\tau) d\tau = \sum_{i=0}^n \beta_i \int_a^b K_{DS(i),y}(t, \tau) y_M(\tau) d\tau
\]
\[
= \int_a^b K_{DS,y}(t, \tau) y_T(\tau) d\tau + \int_a^b K_{DS,y}(t, \tau) \sigma \dot{W}(\tau) d\tau
\] (30)

is a random variable and the following equality holds
\[
y_M(t) = \int_a^b K_{DS,y}(t, \tau) y_M(\tau) d\tau + e(t)
\]
with \( e(t) := \sigma \dot{W}(t) - \int_a^b K_{DS,y}(t, \tau) \sigma \dot{W}(\tau) d\tau \) (33)

since \( y_T \) satisfies the reproducing property in the deterministic regression equation \([14]\). Recall that the annihilator term is subsumed in \( K_{DS,y} \) for convenience of notation.

It is noted that the random error variable \( e \) is dependent on the unknown system parameters \( a_i, i = 0, \cdots, n - 1 \) while the stochastic regression equation
\[
y_M(t) = \sum_{i=0}^n \beta_i \int_a^b K_{DS(i),y}(t, \tau) y_M(\tau) d\tau + e(t)
\] (34)

has the random regressor vector
\[
\left[ \int_a^b K_{DS(0),y}(t, \tau) y_M(\tau) d\tau, \cdots, \int_a^b K_{DS(n),y}(t, \tau) y_M(\tau) d\tau \right]^T
\] (35)

It is easily verified (see later developments) that the assumptions of the Gauss-Markov Theorem are violated in the linear regression problem \([34]\) because the random regressor fails to be homoskedastic. This complication is addressed next.

### 4.1 Heteroskedasticity

Heteroskedasticity has serious consequences for the ordinary least squares (OLS) estimator. Despite that the OLS estimator remains unbiased, the estimated
regression error is wrong while confidence intervals cannot be relied on. A standard quite powerful way to deal with unknown heteroskedasticity is to resort to generalized least squares (GLS), which can be shown to be BLUE (Best Linear Unbiased Estimator); see [43]. The GLS employs inverse covariance weighting in the regression error minimization problem associated with (34).

In similarity with the notation used in the deterministic OLS (18), let $Q(y_M)$ and $P(y_M)$ be the matrices corresponding to $N$ samples of the measurement process realization $y_M$ at a batch of knots $t_1, \ldots, t_N$. Then the stochastic regression error vector is given by

$$e := [e(t_1), \ldots, e(t_N)]^T = Q(y_M) - P(y_M) \bar{a}$$

where $e(t_i)$ are as in (33). The standard GLS regression error minimization for estimation of the parameter vector $\bar{a}$ is

$$\min_{\bar{a}} \left( [Q(y_M) - P(y_M)\bar{a}]^T S [Q(y_M) - P(y_M)\bar{a}] \right)$$

with $S := [\text{Cov}(e)]^{-1}$; $\text{Cov}(e) := E[ee^T]$ (38)

and the components of the covariance matrix calculated as $\text{Cov}(e(t_i), e(t_j))$.

Applying the expectation operator to equations (21) and (33) and using the properties of the Wiener process yields

$$E[y_M(t)] = E[y_T(t)] + \sigma E[\dot{W}(t)] = y_T(t), \quad t \in [a, b]$$

$$E[e(t)] = \sigma E[\dot{W}(t)] - E\left[ \int_a^b K_{DS,y}(t, \tau) \sigma \dot{W}(\tau) d\tau \right] = 0$$

Using the properties (25)–(29) of white noise and recalling that the kernel functions are Hilbert-Schmidt, hence are square integrable, the covariance calculation is then carried out as follows.

$$\text{Cov}[e(t_i), e(t_j)] = E[e(t_i)e(t_j)]$$

$$= \sigma^2 E\left[ \dot{W}(t_i) - \int_a^b K_{DS,y}(t_i, \tau) \dot{W}(\tau) d\tau \right]$$

$$\left[ \dot{W}(t_j) - \int_a^b K_{DS,y}(t_j, s) \dot{W}(s) ds \right]$$

$$= \sigma^2 E[\dot{W}(t_i)\dot{W}(t_j)] - \sigma^2 E\left[ \int_a^b K_{DS,y}(t_i, \tau) \dot{W}(t_j) \dot{W}(\tau) d\tau \right]$$

$$- \sigma^2 E\left[ \int_a^b K_{DS,y}(t_j, s) \dot{W}(t_i) \dot{W}(s) ds \right]$$

$$+ \sigma^2 E\left[ \int_a^b \int_a^b K_{DS,y}(t_i, \tau) K_{DS,y}(t_j, s) \dot{W}(\tau) \dot{W}(s) d\tau ds \right]$$

$$= \sigma^2 \delta(t_i - t_j) - \sigma^2 \int_a^b K_{DS,y}(t_i, \tau) E[\dot{W}(t_j) \dot{W}(\tau)] d\tau$$

14
\[
- \int_a^b K_{DS,y}(t_j, s) E[\dot{W}(t_i)\dot{W}(s)] ds \\
+ \int_a^b \int_a^b K_{DS,y}(t_i, \tau) K_{DS,y}(t_j, s) E[\dot{W}(\tau)\dot{W}(s)] d\tau ds \\
= \sigma^2 \delta(t_i - t_j) - \sigma^2 \int_a^b K_{DS,y}(t_i, \tau) \delta(\tau - t_j) d\tau \\
- \sigma^2 \int_a^b K_{DS,y}(t_j, \tau) \delta(\tau - t_i) d\tau \\
+ \sigma^2 \int_a^b K_{DS,y}(t_i, \tau) \int_a^b K_{DS,y}(t_j, s) \delta(s - \tau) ds d\tau \\
= \sigma^2 \delta(t_i - t_j) - \sigma^2 K_{DS,y}(t_i, t_j) - \sigma^2 K_{DS,y}(t_j, t_i) \\
+ \sigma^2 \int_a^b K_{DS,y}(t_i, \tau) K_{DS,y}(t_j, \tau) d\tau
\]

The formula for the variance follows from (29) and the above:

\[
\text{Var}[e(t)] = \sigma^2 - 2\sigma^2 K_{DS,y}(t, t) + \sigma^2 \int_a^b [K_{DS,y}(t, \tau)]^2 d\tau
\]

At this point it should be clear that the standard GLS as in (37) cannot be applied directly as the covariance matrix depends on the unknown variance \(\sigma^2\) and also on the unknown parameter vector \(\tilde{a}\) in the \(K_{DS,y}\) kernels. Hence a feasible version of the GLS must be employed here in which the covariance matrix is estimated progressively as more information about the regression residuals becomes available. This is typically performed as part of a recursive scheme in which consecutive batches of samples are drawn from the realization of \(y_M\). Letting \(Q_i - P\tilde{a}\) denote the regression error \(e_i\) in batch \(i\), the recursive GLS algorithm computes

\[
\hat{a}_k = \arg \min_{\tilde{a}} \left( \sum_{i=1}^k (Q_i - P\tilde{a})^T S_i (Q_i - P\tilde{a}) \right)
\]

(41)

where \(\hat{a}_k\) is the parameter estimate update at iteration \(k\) of the algorithm. Each weighting matrix \(S_{k+1}\), is calculated as the inverse of the covariance matrix based on the parameter estimate \(\hat{a}_k\) and an estimate of the variance \(\sigma^2\) obtained from the residual trajectory \((y_M(t) - y_E(t))\) in previous iteration \(k\), where \(y_E\) signifies the estimated/reconstructed output; see Appendix D for detailed steps of a modified recursive scheme and initialization of \(S_0\).

At this point it is important to mention that the statistical properties of the feasible GLS are yet not fully known because the algorithm uses successive ‘empirical estimates’ of the covariance matrix and hence relies on large sample properties of the estimation process as a whole.
5 Parametric estimation using multiple regression

The recursive least squares algorithm for parameter estimation can be further improved by using multiple regression equations. Using the reproducing property of kernels in Theorem 1, the kernels are integrated multiple times forming multiple linearly independent regression equations.

For example, consider a fourth order homogeneous LTI system. The kernels are integrated three times to form three additional linearly independent regression equations — four regression equations in total, matching the number of unknown parameters. The formulation of independent regression equations are derived below.

Consider the forward kernel representation (see proof of Theorem 1) for a fourth order homogeneous LTI system:

\[(t - a)^4 y(t) = \int_a^t K\_F,\_y(4, t, \tau) y(\tau)d\tau\] (42)

Integrating both sides of (42) \(n\) times over interval \([a, t]\) and applying Cauchy formula for repeated integration yields

\[
\frac{1}{(n-1)!} \int_a^t (t - \tau)^{n-1}(\tau - a)^4 y(\tau)d\tau = \frac{1}{n!} \int_a^t (t - \tau)^n K\_F,\_y(4, t, \tau) y(\tau)d\tau \quad ; \quad n = 1, 2, 3
\] (43)

\(K\_F,\_y(4, t, \tau)\) can be obtained from Theorem 1 as

\[
K\_F,\_y(4, t, \tau) = 16(\tau - a)^3 - a_3(\tau - a)^4 \\
+ (t - \tau) \left[ - 72(\tau - a)^2 + 12a_3(\tau - a)^3 - a_2(\tau - a)^4 \right] \\
+ \frac{(t - \tau)^2}{2} \left[ 96(\tau - a) - 36a_3(\tau - a)^2 + 8a_2(\tau - a)^3 - a_1(\tau - a)^4 \right] \\
+ \frac{(t - \tau)^3}{6} \left[ - 24 + 24a_3(\tau - a) - 12a_2(\tau - a)^2 + 4a_1(\tau - a)^3 - a_0(\tau - a)^4 \right]
\] (44)

Substituting (44) in (43) yields

\[
\int_a^t (t - \tau)^{n-1}(\tau - a)^4 y(\tau)d\tau = \int_a^t K\_F,\_y^\_n(4, t, \tau) y(\tau)d\tau \quad ; \quad n = 1, 2, 3
\] (45)
where

\[
K_{n,F,y}(4,t,\tau) = \frac{(t-\tau)^n}{n} [16(\tau - a)^3 - a_3(\tau - a)^4]
+ \frac{(t-\tau)^{n+1}}{n} [-72(\tau - a)^2 + 12a_3(\tau - a)^3 - a_2(\tau - a)^4]
+ \frac{(t-\tau)^{n+2}}{2n} [96(\tau - a) - 36a_3(\tau - a)^2 + 8a_2(\tau - a)^3 - a_1(\tau - a)^4]
+ \frac{(t-\tau)^{n+3}}{6n} [-24 + 24a_3(\tau - a) - 12a_2(\tau - a)^2 + 4a_1(\tau - a)^3 - a_0(\tau - a)^4]
\]

Similarly, consider the backward kernel representation (see proof of Theorem 1) for a fourth order homogeneous LTI system:

\[
(b - t)^4 y(t) = \int_t^b K_{B,y}(4,t,\tau) y(\tau) d\tau \tag{47}
\]

Integrating both sides of \(47\) \(n\) times over interval \([t,b]\) and applying Cauchy formula for repeated integration yields

\[
\frac{1}{(n-1)!} \int_t^b (t-\tau)^{n-1}(b - \tau)^4 y(\tau) d\tau = \frac{-1}{n!} \int_t^b (t-\tau)^n K_{B,y}(4,t,\tau) y(\tau) d\tau ; \ n = 1, 2, 3 \tag{48}
\]

\(K_{B,y}(4,t,\tau)\) can be obtained from Theorem 1 as

\[
K_{B,y}(4,t,\tau) = 16(b - \tau)^3 + a_3(b - \tau)^4
+ (t - \tau) \left[72(b - \tau)^2 + 12a_3(b - \tau)^3 + a_2(b - \tau)^4 \right]
+ \frac{(t-\tau)^2}{2} \left[96(b - \tau) + 36a_3(b - \tau)^2 + 8a_2(b - \tau)^3 + a_1(b - \tau)^4 \right]
+ \frac{(t-\tau)^3}{6} \left[24 + 24a_3(b - \tau) + 12a_2(b - \tau)^2 + 4a_1(b - \tau)^3 + a_0(b - \tau)^4 \right] \tag{49}
\]

Substituting \(49\) in \(48\) yields

\[
\int_t^b (t-\tau)^{n-1}(b - \tau)^4 y(\tau) d\tau = \int_t^b K_{B,y}^n(4,t,\tau) y(\tau) d\tau ; \ n = 1, 2, 3 \tag{50}
\]
where

\[ K_{B,y}^n(4,t,\tau) = \frac{-(t-\tau)^n}{n} \left[ 16(b-\tau)^3 + a_3(b-\tau)^4 \right] \]

\[ - \frac{(t-\tau)^{n+1}}{n} \left[ 72(b-\tau)^2 + 12a_3(b-\tau)^3 + a_2(b-\tau)^4 \right] \]

\[ - \frac{(t-\tau)^{n+2}}{2n} \left[ 96(b-\tau) + 36a_3(b-\tau)^2 + 8a_2(b-\tau)^3 + a_1(b-\tau)^4 \right] \]

\[ - \frac{(t-\tau)^{n+3}}{6n} \left[ 24 + 24a_3(b-\tau) + 12a_2(b-\tau)^2 + 4a_1(b-\tau)^3 + a_0(b-\tau)^4 \right] \]  

Adding equations (45) and (50) yields the three additional linearly independent regression equations for a fourth order homogeneous LTI system as

\[ \int_a^b (t-\tau)^{n-1} \alpha(4,t,\tau) y(\tau) \, d\tau = \int_a^b K_{DS,y}^n(4,t,\tau) y(\tau) \, d\tau \quad ; \quad n = 1, 2, 3 \]  

with

\[ \alpha(4,t,\tau) \triangleq \begin{cases} (\tau - a)^4, & \text{for } \tau \leq t \\ (b - \tau)^4, & \text{for } \tau > t \end{cases} \]  

\[ K_{DS,y}^n(4,t,\tau) \triangleq \begin{cases} K_{F,y}^n(4,t,\tau), & \text{for } \tau \leq t \\ K_{B,y}^n(4,t,\tau), & \text{for } \tau > t \end{cases} \]  

The treatment applied in Section 4 is repeated here for the four linearly independent regression equations for a fourth order homogeneous LTI system:

\[ [(t - a)^4 + (b - t)^4] y(t) = \sum_{i=0}^{n} \beta_i \int_a^b K_{DS(i),y}^i(4,t,\tau) y(\tau) \, d\tau \]  

\[ \int_a^b \alpha(4,t,\tau) y(\tau) \, d\tau = \sum_{i=0}^{n} \beta_i \int_a^b K_{DS(i),y}^i(4,t,\tau) y(\tau) \, d\tau \]  

\[ \int_a^b (t-\tau) \alpha(4,t,\tau) y(\tau) \, d\tau = \sum_{i=0}^{n} \beta_i \int_a^b K_{DS(i),y}^i(4,t,\tau) y(\tau) \, d\tau \]  

\[ \int_a^b (t-\tau)^2 \alpha(4,t,\tau) y(\tau) \, d\tau = \sum_{i=0}^{n} \beta_i \int_a^b K_{DS(i),y}^i(4,t,\tau) y(\tau) \, d\tau \]  

where \( K_{DS(i),y}; i = 0, \ldots, n \) and \( K_{DS(i),y}^n; i = 0, \ldots, n \) are respectively the ‘component kernels’ of \( K_{DS,y} \) and \( K_{DS,y}^n \), that post-multiply the coefficients \( \beta_i = a_i; i = 0, \ldots, n \), with \( \beta_n = a_n = 1 \) for convenience of notation. Note that unlike Section 4, here the annihilator term is not subsumed in \( K_{DS} \).

In a noise-free deterministic setting, the output variable \( y \) becomes the measured output coinciding with the nominal output trajectory \( y_T \), so the regression
equations (55)–(58) for the constant parameters \(a_i, i = 0, \ldots, n-1\), can be written in a partitioned form as

\[
\left[(t-a)^4 + (b-t)^4\right] y_T(t) = [K_{\bar{a}}, K_{a_n}](t; y_T) \beta
\]

\[
\int_a^b \alpha(4, t, \tau) y_T(\tau) \, d\tau = [K_{\bar{a}}, K_{a_n}](t; y_T) \beta
\]

\[
\int_a^b (t-\tau) \alpha(4, t, \tau) y_T(\tau) \, d\tau = [K_{\bar{a}}, K_{a_n}](t; y_T) \beta
\]

\[
\int_a^b (t-\tau)^2 \alpha(4, t, \tau) y_T(\tau) \, d\tau = [K_{\bar{a}}, K_{a_n}](t; y_T) \beta
\]

with

\[
\bar{a} := [a_0; \cdots; a_{n-1}] \quad \beta := [\bar{a} ; 1]
\]

where \(K_{\bar{a}}(t; y_T), K_{a_0}^1(t; y_T), K_{a_0}^2(t; y_T), \) and \(K_{a_0}^3(t; y_T)\) are row vectors with corresponding integral components:

\[
K_{\bar{a}}(t; y_T)_k := \int_a^b K_{DS(k,y)}(4, t, \tau) y_T(\tau) \, d\tau \quad k = 0, \ldots, n-1
\]

\[
K_{a_0}^1(t; y_T)_k := \int_a^b K_{DS(k,y)}^1(4, t, \tau) y_T(\tau) \, d\tau \quad k = 0, \ldots, n-1
\]

\[
K_{a_0}^2(t; y_T)_k := \int_a^b K_{DS(k,y)}^2(4, t, \tau) y_T(\tau) \, d\tau \quad k = 0, \ldots, n-1
\]

\[
K_{a_0}^3(t; y_T)_k := \int_a^b K_{DS(k,y)}^3(4, t, \tau) y_T(\tau) \, d\tau \quad k = 0, \ldots, n-1
\]

while \(K_{a_n}(t; y_T), K_{a_n}^1(t; y_T), K_{a_n}^2(t; y_T), \) and \(K_{a_n}^3(t; y_T)\) are scalars

\[
K_{a_n}(t; y_T) := \int_a^b K_{DS(n,y)}(4, t, \tau) y_T(\tau) \, d\tau
\]

\[
K_{a_n}^1(t; y_T) := \int_a^b K_{DS(n,y)}^1(4, t, \tau) y_T(\tau) \, d\tau
\]

\[
K_{a_n}^2(t; y_T) := \int_a^b K_{DS(n,y)}^2(4, t, \tau) y_T(\tau) \, d\tau
\]

\[
K_{a_n}^3(t; y_T) := \int_a^b K_{DS(n,y)}^3(4, t, \tau) y_T(\tau) \, d\tau
\]

corresponding to \(a_n = 1\).

Re-arranging the terms, the equations (59)–(62) can be written in matrix form as

\[
\begin{bmatrix}
[t(t-a)^4 + (b-t)^4] y_T(t) - K_{a_n}(t; y_T) \\
\int_a^b \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^1(t; y_T) \\
\int_a^b (t-\tau) \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^2(t; y_T) \\
\int_a^b (t-\tau)^2 \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^3(t; y_T)
\end{bmatrix} =
\begin{bmatrix}
K_{\bar{a}}(t; y_T) \\
K_{\bar{a}}^1(t; y_T) \\
K_{\bar{a}}^2(t; y_T) \\
K_{\bar{a}}^3(t; y_T)
\end{bmatrix}
\]

\[
\begin{bmatrix}
K_{\bar{a}}(t; y_T) \\
K_{\bar{a}}^1(t; y_T) \\
K_{\bar{a}}^2(t; y_T) \\
K_{\bar{a}}^3(t; y_T)
\end{bmatrix} = 
\begin{bmatrix}
K_{a_n}(t; y_T) \\
K_{a_n}^1(t; y_T) \\
K_{a_n}^2(t; y_T) \\
K_{a_n}^3(t; y_T)
\end{bmatrix}
\]
Defining

\[ q^0(t; y_T) := [(t-a)^4 + (b-t)^4] y_T(t) - K_{a_n}(t; y_T) \] (73)

\[ q^1(t; y_T) := \int_a^b \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^1(t; y_T) \] (74)

\[ q^2(t; y_T) := \int_a^b (t-\tau) \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^2(t; y_T) \] (75)

\[ q^3(t; y_T) := \int_a^b (t-\tau)^2 \alpha(4, t, \tau) y_T(\tau) \, d\tau - K_{a_n}^3(t; y_T) \] (76)

\[ p^0(t; y_T) := K_a(t; y_T) \] (77)

\[ p^1(t; y_T) := K_a^1(t; y_T) \] (78)

\[ p^2(t; y_T) := K_a^2(t; y_T) \] (79)

\[ p^3(t; y_T) := K_a^3(t; y_T) \] (80)

and given distinct time instants \( t_1, \ldots, t_N \in (a, b) \), here referred to as knots, the matrix equation (72) is re-written point-wise in the form of another matrix equation:

\[ Q(y_T) = P(y_T)\tilde{a} \] (81)

where

\[ Q(y_T) := \begin{bmatrix} \tilde{q}^0(y_T) \\ \tilde{q}^1(y_T) \\ \tilde{q}^2(y_T) \\ \tilde{q}^3(y_T) \end{bmatrix} ; \quad P(y_T) := \begin{bmatrix} \tilde{p}^0(y_T) \\ \tilde{p}^1(y_T) \\ \tilde{p}^2(y_T) \\ \tilde{p}^3(y_T) \end{bmatrix} \]

with

\[ \tilde{q}^i(y_T) := \begin{bmatrix} q^i(t_1; y_T) \\ \vdots \\ q^i(t_N; y_T) \end{bmatrix} ; \quad i = 0, 1, 2, 3 \]

and

\[ \tilde{p}^i(y_T) := \begin{bmatrix} p^i(t_1; y_T) \\ \vdots \\ p^i(t_N; y_T) \end{bmatrix} ; \quad i = 0, 1, 2, 3 \]

Clearly, \( Q \in \mathbb{R}^{nN} \) and \( P \in \mathbb{R}^{nN} \times \mathbb{R}^n \) while \( \tilde{a} \in \mathbb{R}^n \) (here, \( n = 4 \) for the fourth order example).

Equation (81) can be solved using least squares error minimization provided adequate identifiability assumptions are met; see Definition 2.

Let a given noisy realization of the observed system output \( y_M(t), t \in [a, b] \), be persistent and the observation noise be white Gaussian and additive. In search for the knots for which identifiability holds and to compensate for the noise, the search for the system parameters \( \tilde{a} \) is best solved by way of a recursive least-square regression algorithm — as described in Section 4.1.
5.1 Error covariance matrices

Following the stochastic treatment applied in Section 4, the matrix regression equation (81) can be modified as:

\[ Q(y_M) = P(y_M)\bar{a} + e \]  

where

\[ e := \begin{bmatrix} e^0 \\ e^1 \\ e^2 \\ e^3 \end{bmatrix} \quad \text{and} \quad \bar{e}^i := \begin{bmatrix} e^i(t_1) \\ \vdots \\ e^i(t_N) \end{bmatrix} \quad ; \quad i = 0, 1, 2, 3 \]

with

\[ e^0(t) = [(t - a)^4 + (b - t)^4] \sigma \dot{W}(t) - \sigma \int_a^b K_{DS,y}(4, t, \tau) \dot{W}(\tau) \, d\tau \]  

\[ e^1(t) = \sigma \int_a^b (t - \tau) \alpha(4, t, \tau) \dot{W}(\tau) \, d\tau - \sigma \int_a^b K_{DS,y}^1(4, t, \tau) \dot{W}(\tau) \, d\tau \]  

\[ e^2(t) = \sigma \int_a^b (t - \tau)^2 \alpha(4, t, \tau) \dot{W}(\tau) \, d\tau - \sigma \int_a^b K_{DS,y}^2(4, t, \tau) \dot{W}(\tau) \, d\tau \]  

\[ e^3(t) = \sigma \int_a^b (t - \tau)^2 \alpha(4, t, \tau) \dot{W}(\tau) \, d\tau - \sigma \int_a^b K_{DS,y}^3(4, t, \tau) \dot{W}(\tau) \, d\tau \]

As explained in Section 4.1, the regression error minimization problem associated with (82) is solved using generalized least squares (GLS) by employing inverse covariance weighting. The standard GLS regression error minimization for estimation of the parameter vector \( \bar{a} \) is

\[ \min_{\bar{a}} \left( [Q(y_M) - P(y_M)\bar{a}]^T S [Q(y_M) - P(y_M)\bar{a}] \right) \]  

with the weighting matrix \( S \in \mathbb{R}^{nN} \times \mathbb{R}^{nN} \) defined as

\[ S := \text{diag}(S^0, S^1, \ldots, S^{n-1}) \]  

where the matrices \( S^i \in \mathbb{R}^{N} \times \mathbb{R}^{N} ; i = 0, \ldots, n - 1 \) are the inverses of corresponding error covariance matrices, as given by:

\[ [S^i]^{-1} = \begin{bmatrix} \text{Cov}[e^i(t_1), e^i(t_1)] & \cdots & \text{Cov}[e^i(t_1), e^i(t_N)] \\ \vdots & \ddots & \vdots \\ \text{Cov}[e^i(t_N), e^i(t_1)] & \cdots & \text{Cov}[e^i(t_N), e^i(t_N)] \end{bmatrix} \quad ; \quad i = 0, \ldots, n - 1 \]

Components of the error covariance matrices are calculated as shown below. Following the treatment applied in Section 4.1 and using the properties of the Wiener process yields

\[ \mathbb{E}[e^i(t)] = 0 \quad ; \quad i = 0, 1, 2, 3 \]  

21
\[ \text{Cov}[e^0(t_i), e^0(t_j)] = E[e^0(t_i) e^0(t_j)] \]
\[ = \sigma^2 E \left[ \left[ (t_i - a)^4 + (b - t_i)^4 \right] \hat{W}(t_i) - \int_a^b K_{DS,y}(4, t_i, \tau) \hat{W}(\tau) \, d\tau \right] \]
\[ \left[ (t_j - a)^4 + (b - t_j)^4 \right] \hat{W}(t_j) - \int_a^b K_{DS,y}(4, t_j, s) \hat{W}(s) \, ds \right] \]
\[ = \sigma^2 \left[ (t_i - a)^4 + (b - t_i)^4 \right] \left[ (t_j - a)^4 + (b - t_j)^4 \right] E[\hat{W}(t_i) \hat{W}(t_j)] \]
\[ - \left[ (t_i - a)^4 + (b - t_i)^4 \right] \int_a^b K_{DS,y}(4, t_i, s) E[\hat{W}(t_i) \hat{W}(s)] \, ds \]
\[ - \left[ (t_j - a)^4 + (b - t_j)^4 \right] \int_a^b K_{DS,y}(4, t_j, \tau) E[\hat{W}(t_j) \hat{W}(\tau)] \, d\tau \]
\[ + \int_a^b \int_a^b K_{DS,y}(4, t_i, \tau) K_{DS,y}(4, t_j, \tau) E[\hat{W}(\tau) \hat{W}(s)] \, d\tau \, ds \]
\[ = \sigma^2 \left[ (t_i - a)^4 + (b - t_i)^4 \right] \left[ (t_j - a)^4 + (b - t_j)^4 \right] \delta(t_i - t_j) \]
\[ - \left[ (t_i - a)^4 + (b - t_i)^4 \right] K_{DS,y}(4, t_i, t_i) \]
\[ - \left[ (t_j - a)^4 + (b - t_j)^4 \right] K_{DS,y}(4, t_i, t_j) \]
\[ + \int_a^b K_{DS,y}(4, t_i, \tau) K_{DS,y}(4, t_j, \tau) \, d\tau \] (91)

\[ \text{Cov}[e^1(t_i), e^1(t_j)] = E[e^1(t_i) e^1(t_j)] \]
\[ = \sigma^2 E \left[ \int_a^b \alpha(4, t_i, \tau) \hat{W}(\tau) \, d\tau - \int_a^b K_{DS,y}^1(4, t_i, \tau) \hat{W}(\tau) \, d\tau \right] \]
\[ \left[ \int_a^b \alpha(4, t_j, s) \hat{W}(s) \, ds - \int_a^b K_{DS,y}^1(4, t_j, s) \hat{W}(s) \, ds \right] \]
\[ = \sigma^2 \left[ \int_a^b \int_a^b \alpha(4, t_i, \tau) \alpha(4, t_j, s) E[\hat{W}(\tau) \hat{W}(s)] \, d\tau \, ds \right] \]
\[ - \int_a^b \int_a^b \alpha(4, t_i, \tau) K_{DS,y}^1(4, t_i, s) E[\hat{W}(\tau) \hat{W}(s)] \, d\tau \, ds \]
\[ - \int_a^b \int_a^b \alpha(4, t_j, s) K_{DS,y}^1(4, t_i, \tau) E[\hat{W}(\tau) \hat{W}(s)] \, d\tau \, ds \]
\[ + \int_a^b \int_a^b K_{DS,y}^1(4, t_i, \tau) K_{DS,y}^1(4, t_j, s) E[\hat{W}(\tau) \hat{W}(s)] \, d\tau \, ds \]
\[ = \sigma^2 \left[ \int_a^b \alpha(4, t_i, \tau) \alpha(4, t_j, \tau) \, d\tau - \int_a^b \alpha(4, t_i, \tau) K_{DS,y}^1(4, t_j, \tau) \, d\tau \right] \]
\[
- \int_a^b \alpha(4, t_j, \tau) K_{DS,y}^1(4, t_i, \tau) \, d\tau \\
+ \int_a^b K_{DS,y}^1(4, t_i, \tau) K_{DS,y}^2(4, t_j, \tau) \, d\tau
\]

\[
\text{Cov}[e^2(t_i), e^2(t_j)] = \text{E}[e^2(t_i) e^2(t_j)]
\]

\[
= \sigma^2 \left[ \int_a^b (t_i - \tau) \alpha(4, t_i, \tau) W(\tau) \, d\tau - \int_a^b K_{DS,y}^2(4, t_i, \tau) \dot{W}(\tau) \, d\tau \right]
\]

\[
\text{Cov}[e^3(t_i), e^3(t_j)] = \text{E}[e^3(t_i) e^3(t_j)]
\]

\[
= \sigma^2 \left[ \int_a^b (t_i - \tau)^2 \alpha(4, t_i, \tau) W(\tau) \, d\tau - \int_a^b K_{DS,y}^2(4, t_i, \tau) \dot{W}(\tau) \, d\tau \right]
\]
\[
+ \int_{a}^{b} \int_{a}^{b} K_{DS,y}^{3}(4, t_i, \tau) K_{DS,y}^{3}(4, t_j, s) \ E[\dot{W}(\tau) \dot{W}(s)] \ d\tau \ ds
\]

\[= \sigma^2 \left[ \int_{a}^{b} (t_i - \tau)^2 (t_j - \tau)^2 \alpha(4, t_i, \tau) \alpha(4, t_j, \tau) \ d\tau \\
- \int_{a}^{b} (t_i - \tau)^2 \alpha(4, t_i, \tau) K_{DS,y}^{3}(4, t_j, \tau) \ d\tau \\
- \int_{a}^{b} (t_j - \tau)^2 \alpha(4, t_j, \tau) K_{DS,y}^{3}(4, t_i, \tau) \ d\tau \\
+ \int_{a}^{b} K_{DS,y}^{3}(4, t_i, \tau) K_{DS,y}^{3}(4, t_j, \tau) \ d\tau \right] \tag{94}
\]

Note that here the annihilator term is not subsumed in $K_{DS,y}$ — hence the difference in the covariance terms with those in Section 4.1.

As mentioned in Section 4.1, it is clear that the standard GLS as in (87) cannot be applied directly as the covariance matrices depend on the unknown variance $\sigma^2$ and also on the unknown parameter vector $\bar{a}$ in the $K_{DS,y}$ kernels. Hence a feasible version of the GLS is employed in which the covariance matrices are estimated progressively as more information about the multiple regression residuals becomes available. This is typically performed as part of a recursive scheme in which consecutive batches of samples are drawn from the realization of $y_M$ — as explained in Section 4.1.

6 Trajectory and derivative reconstruction

Once the parameters of the system are estimated successfully, the system output can be reconstructed by projection onto the finite dimensional subspace of the RKHS spanned by the fundamental solutions of the characteristic equation, here denoted by $\xi_1, \cdots, \xi_n$: refer to Corollary 1. The fundamental solutions are found by integrating the characteristic equation for $n$ sets of initial conditions:

\[Y(0)_k := [y(0), y^{(1)}(0), \cdots, y^{(n-1)}(0)] = B_k; \quad k = 1, \cdots, n \tag{95}\]

where $B_k$ are the canonical basis vectors in $\mathbb{R}^n$. For efficiency of computations it makes sense to orthonormalize the set $\xi_k, k = 1, \cdots, n$ into $\zeta_k, k = 1, \cdots, n$, using the Gram-Schmidt orthonormalization procedure in $L^2$. As the orthonormalizing transformation is linear

\[
\text{span}\{\xi_k, k = 1, \cdots, n\} = \text{span}\{\zeta_k, k = 1, \cdots, n\} := \Xi \\
\langle \zeta_i | \zeta_j \rangle_2 = 0, i \neq j; \quad \langle \zeta_i | \zeta_i \rangle_2 = 1 \tag{96}\]

with $\langle \cdot | \cdot \rangle_2$ as the inner product in $L^2$. Since the noise-free output to be estimated is a linear combination of fundamental solutions

\[y_T = \sum_{i=1}^{n} c_i \zeta_i; \quad \text{with} \quad c_i = \langle y_T | \zeta_i \rangle_2, \quad i = 1, \cdots, n \tag{97}\]

24
it is natural to consider a similar form for the estimator $\hat{y}_T$ with linear estimators $\hat{c}_i$ for the coefficients $c_i$ in the form

$$\hat{c}_i := \langle y_M | \zeta_i \rangle_2 = \int_a^b y_M(\tau)\zeta_i(\tau) d\tau, \quad i = 1, \cdots, n \quad (98)$$

The above are in fact unbiased MMSE estimators for the coefficients of $\hat{y}_T$ which is verified immediately by using (29) while defining the estimation error $\bar{e}^c$:

$$\bar{e}^c := [\bar{e}^{c1}, \cdots, \bar{e}^{cn}]; \quad \bar{e}^{ci} := \langle y_M | \zeta_i \rangle_2 - \langle y_T | \zeta_i \rangle_2, \quad i = 1, \cdots, n$$

$$E[\bar{e}^{ci}] = E \int_a^b \sigma \hat{W}(\tau)\zeta_i(\tau) d\tau = 0 \quad (99)$$

which proves unbiasedness. The estimator variances are calculated as follows, also using (29):

$$E[(e^{ci})^2] = E \left( \int_a^b \sigma \hat{W}(\tau)\zeta_i(\tau) d\tau \right)^2 = \sigma^2 \int_a^b \zeta_i^2(\tau) d\tau = \sigma^2, \quad i = 1, \cdots, n \quad (100)$$

The resulting estimator $\hat{y}_T$ using the coefficients of (98) is also BLUE because it can be viewed as an OLS in which a set of measurements $y_M$ is projected onto a given subspace $\Xi$ where the measurement errors are Gaussian i.i.d. hence satisfying the strict Gauss-Markov assumptions.

To conclude, given a measurement process realization $\bar{y}_M$ on $[a, b]$, the reconstructed output trajectory is obtained as

$$y_E(t) = \sum_{i=1}^n \langle \bar{y}_M | \zeta_i \rangle_2 \zeta_i(t); \quad t \in [a, b] \quad (101)$$

The estimates of the derivatives $y_E^{(i)}, i = 1, \cdots, n - 1$ are obtained by way of integral transforms of $y_E$ with the kernels of Theorem 2.

Finally, it should be mentioned (see also Remark 1) that trajectory reconstruction can be performed directly in the ‘feature space’ (12), i.e. in the basis provided by the ‘feature spline’ functions represented by kernels $K_{DS,y}(t_i, \cdot)$ at a selection of knots $t_i, i = 1, \cdots, N$ in place of fundamental solutions $\zeta_i$. In this case $N$ should be sufficiently large to obtain comparable accuracy of results.

7 Results

An unstable 4-th order system is considered with characteristic equation

$$y^{(4)}(t) + a_3y^{(3)}(t) + a_2y^{(2)}(t) + a_1y^{(1)}(t) + a_0y(t) = 0 \quad (102)$$

where the nominal values of parameters are

$$a_0 = 1, \quad a_1 = 5, \quad a_2 = 5, \quad a_3 = 0 \quad (103)$$
The following initial values are used:
\[ y(0) = 3, \quad y^{(1)}(0) = -2, \quad y^{(2)} = 5, \quad y^{(3)} = 7 \]  
(104)

The measured realization of the output \( y_M \) is obtained as \( y_M = y_T + \sigma \hat{W} \) with \( \sigma = 13 \) and \( \sigma = 20 \).

For \( \sigma = 13 \), the signal-to-noise ratio is 0.1180, or equivalently -9.2826 dB. Figure 1 shows \( y_M \) vs \( y_T \) for this level of noise. The recursive feasible GLR is employed in batches of \( N = 125, N = 250, \) and \( N = 500 \) knots sampled from a uniform distribution over \([a, b] = [0, 6]\). The final parameter estimates are shown in Table 1. The parameter estimates do not improve further beyond the number of samples \( N = 500 \), most probably due to accumulation of numerical errors. The estimated/reconstructed output trajectories and their derivatives: \( y_E, y_E^{(1)}, y_E^{(2)}, y_E^{(3)} \), are calculated as explained in Section 6. Figures 2, 3, 4, 5 show \( y_E, y_E^{(1)}, y_E^{(2)}, y_E^{(3)} \), respectively, using the estimated parameter values for \( N = 500 \).

The performance of the estimation approach is further tested with an increased measurement noise level (AWGN with standard deviation of \( \sigma = 20 \)) which correspond to signal-to-noise ratio of 0.0499, or in decibel scale: -13.0218 dB. Figure 6 shows \( y_M \) vs \( y_T \) for this level of noise. The final parameter estimates are shown in Table 1. The parameter estimates do not improve further beyond the number of samples \( N = 750 \). Figures 7, 8, 9, 10 show the estimated/reconstructed output trajectories and their derivatives: \( y_E, y_E^{(1)}, y_E^{(2)} \),
Figure 2: Reconstructed $y_E$ from noise of 13 SD (SNR -9.2826 dB)

Figure 3: Reconstructed $y^{(1)}_E$ from noise of 13 SD (SNR -9.2826 dB)
Figure 4: Reconstructed $y_E^{(2)}$ from noise of 13 SD (SNR -9.2826 dB)

Figure 5: Reconstructed $y_E^{(3)}$ from noise of 13 SD (SNR -9.2826 dB)
Figure 6: Noisy $y_M$ vs nominal $y_T$ for noise of 20 SD (SNR -13.0218 dB)

$y_E^{(3)}$, respectively.

The standard root mean square deviation (RMSD) is used to assess proximity of the nominal and estimated/reconstructed trajectories $y_T$ and $y_E$.

For improved quantitative evaluation of the estimation accuracy, the estimation error is also assessed in terms of the Sobolev norm in $W^{3}_{\infty}$; i.e.

$$
\text{Maximum absolute difference (MAD)} = \max_{t \in [a, b]} \left( \sum_{k=0}^{3} |y_E^{(k)}(t) - y_T^{(k)}(t)| \right)
$$

(105) that penalizes deviations in the first three estimated derivatives $y_E^{(i)}$, $i = 1, 2, 3$ also. The minimum and maximum of the error values over the interval $[a, b]$ are recorded at time instants

$$
t_* = \arg \min_{t \in [a, b]} \left( \sum_{k=0}^{3} |y_E^{(k)}(t) - y_T^{(k)}(t)| \right)
$$

(106)

$$
t^* = \arg \max_{t \in [a, b]} \left( \sum_{k=0}^{3} |y_E^{(k)}(t) - y_T^{(k)}(t)| \right)
$$

(107)

The knowledge of $t_*$ and $t^*$ is useful as the first one can be used to provide ‘a launch pad’ for extrapolation as the phase-space point $[y_E, y_E^{(1)}, \cdots, y_E^{(1)}](t_*)$ while the $t^*$ indicates areas for potential accuracy improvement e.g. by adding knots in the regression equations.
Figure 7: Reconstructed $y_E$ from noise of 20 SD (SNR -13.0218 dB)

Figure 8: Reconstructed $y_E^{(1)}$ from noise of 20 SD (SNR -13.0218 dB)
Figure 9: Reconstructed $y^{(2)}_E$ from noise of 20 SD (SNR -13.0218 dB)

Figure 10: Reconstructed $y^{(3)}_E$ from noise of 20 SD (SNR -13.0218 dB)
Table 1: Estimated parameter values

| Noise | Values | $a_0$ | $a_1$ | $a_2$ | $a_3$ |
|-------|--------|-------|-------|-------|-------|
| True  |        | 1     | 5     | 5     | 0     |
| $\sigma = 13$ | Estimated |         | 0.9320 | 4.8078 | 5.1724 | 0.1342 |
|        | (N = 125) |       |       |       |       |
| $\sigma = 13$ | Estimated |         | 0.9795 | 5.0203 | 4.9891 | 0.0031 |
|        | (N = 250) |       |       |       |       |
| $\sigma = 13$ | Estimated |         | 0.9798 | 4.9892 | 5.0075 | 0.0020 |
|        | (N = 500) |       |       |       |       |
| $\sigma = 20$ | Estimated |         | 0.5107 | 4.2814 | 5.1336 | -0.2151 |
|        | (N = 750) |       |       |       |       |

Table 2: Calculated error metrics for the estimated trajectories

| Noise | Samples | RMSD  | Estimated $\sigma$ | MAD  | $t_*$  | $t^*$ |
|-------|---------|-------|---------------------|------|--------|------|
| $\sigma = 13$ | $N = 125$ | 0.4055 | 13.0373 | 17.9944 | 4.9689 | 5.6724 |
| $\sigma = 13$ | $N = 250$ | 0.1098 | 12.9599 | 5.4473 | 1.2709 | 6.0 |
| $\sigma = 13$ | $N = 500$ | 0.0692 | 12.9993 | 1.2702 | 0.6603 | 6.0 |
| $\sigma = 20$ | $N = 750$ | 0.1510 | 20.0161 | 18.9594 | 0.0 | 6.0 |

Table 2 shows the calculated error metrics for the estimated trajectories for the different cases considered.

Discussion of results:
The reconstructed output and derivative trajectories are virtually indistinguishable from their nominal counterparts for a measurement process realization with SNR -9.2826 dB (as evident from Figures 2-5), and even with the noise of SNR -13.0218 dB, the estimates are remarkably close to their true counterparts (as seen in Figures 7-10).

7.1 Comparison with Unscented Rauch-Tung-Striebel smoother

The presented method is compared to the Unscented Rauch-Tung-Striebel (URTS) smoother [28], [29]. The comparison is carried out for both noise levels of standard deviation $\sigma = 13$ (signal-to-noise ratio -9.2826 dB) and standard deviation $\sigma = 20$ (signal-to-noise ratio -13.0218 dB).

For simultaneous state and parameter estimation using the URTS smoother, the state and parameters of the 4th order LTI system are combined to form a new aggregated state vector:

$$[x_1 \ x_2 \ x_3 \ x_4 \ a_0 \ a_1 \ a_2 \ a_3]^T \quad (108)$$
The dynamics of this new extended 8th order nonlinear model are:

\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\dot{x}_3 \\
\dot{x}_4 \\
\dot{a}_0 \\
\dot{a}_1 \\
\dot{a}_2 \\
\dot{a}_3
\end{bmatrix} =
\begin{bmatrix}
x_2 \\
x_3 \\
x_4 \\
-a_0 x_1 - a_1 x_2 - a_2 x_3 - a_3 x_4 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\]  
(109)

\[
y =
\begin{bmatrix}
1^T \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
a_0 \\
a_1 \\
a_2 \\
a_3
\end{bmatrix}
\]  
(110)

The Unscented RTS smoother (based on the Unscented Kalman filter) is applied on this 8th order nonlinear model for the given window of noisy measurements. For the Unscented transform, sigma points and weights are generated according to [44]. It parameterizes the sigma points using alpha, beta, kappa terms, and is the version seen in most publications. Alpha determines the spread of the sigma points around the mean; usually a small positive value is taken. Beta incorporates prior knowledge of the distribution of the mean. For Gaussian states, beta = 2 is optimal. Kappa is a secondary scaling parameter, usually set to 0. The values of the parameters used are:

\[
\alpha = 0.001, \quad \beta = 2, \quad \kappa = 0
\]  
(111)

The initial state values supplied are: \( \begin{bmatrix} 0, 0, 0, 0, 0, 0, 0, 0 \end{bmatrix}^T \)

The true values of the measurement noise variances are given to the URTS smoother. It should be noted that, unlike the URTS smoother, the kernel estimation or the subsequent trajectory reconstruction method presented in this paper does not require the knowledge of the noise variance.

Figure 11 shows the comparison of the \( y \) trajectory reconstructed via the projection method and that obtained from the URTS smoother, while Figures 12, 13, 14 show the comparisons of \( y^{(1)}_E, y^{(2)}_E, y^{(3)}_E \), respectively — for the noise level of standard deviation \( \sigma = 13 \) (signal-to-noise ratio -9.2826 dB). Figures 15, 16, 17, 18 show the corresponding comparisons for the noise level of standard deviation \( \sigma = 20 \) (signal-to-noise ratio -13.0218 dB). Table 3 shows the comparison of the estimated parameter values. Table 4 shows the comparison of the estimated trajectories via relevant error metrics introduced earlier.

As it is clear from Figures 11, 15, and Tables 3 & 4, the estimations obtained through projection and kernel method are superior to those obtained from the
Figure 11: Comparison of reconstructed $y_E$ from noise of 13 SD (SNR -9.2826 dB)

Figure 12: Comparison of reconstructed $y^{(1)}_E$ from noise of 13 SD (SNR -9.2826 dB)
Figure 13: Comparison of reconstructed $y_E^{(2)}$ from noise of 13 SD (SNR -9.2826 dB)

Figure 14: Comparison of reconstructed $y_E^{(3)}$ from noise of 13 SD (SNR -9.2826 dB)
Figure 15: Comparison of reconstructed $y_E$ from noise of 20 SD (SNR -13.0218 dB)

Figure 16: Comparison of reconstructed $y_E^{(1)}$ from noise of 20 SD (SNR -13.0218 dB)
Figure 17: Comparison of reconstructed $y_E^{(2)}$ from noise of 20 SD (SNR -13.0218 dB)

Figure 18: Comparison of reconstructed $y_E^{(3)}$ from noise of 20 SD (SNR -13.0218 dB)
Table 3: Comparison of estimated parameter values

| Noise | Values | \( a_0 \) | \( a_1 \) | \( a_2 \) | \( a_3 \) |
|-------|--------|-------------|-------------|-------------|-------------|
| True  |        | 1           | 5           | 5           | 0           |
| \( \sigma = 13 \) | Estimated via proposed method \((N = 500)\) | 0.9798 | 4.9892 | 5.0075 | 0.0020 |
| \( \sigma = 13 \) | Estimated via URTS smoother | 0.1051 | -0.6286 | 7.3110 | -3.6655 |
| \( \sigma = 20 \) | Estimated via proposed method \((N = 750)\) | 0.5107 | 4.2814 | 5.1336 | -0.2151 |
| \( \sigma = 20 \) | Estimated via URTS smoother | -0.1306 | -2.0833 | 5.8567 | -3.9354 |

Table 4: Comparison of estimated trajectories via error metrics

| Noise | Method | RMSD | MAD  |
|-------|--------|------|------|
| \( \sigma = 13 \) | Estimated via proposed method \((N = 500)\) | 0.0692 | 1.2702 |
| \( \sigma = 13 \) | Estimated via URTS smoother | 0.6449 | 349.1531 |
| \( \sigma = 20 \) | Estimated via proposed method \((N = 750)\) | 0.1510 | 18.9594 |
| \( \sigma = 20 \) | Estimated via URTS smoother | 1.0876 | 795.8028 |
URTS smoother. As noted earlier, unlike the URTS smoother, the proposed estimation method does not require the knowledge of the noise variance.

8 Conclusion

The results presented here consider estimation of linear systems from a slightly different perspective. From a point of view of prediction, it is not the discerning of the shape of the observed trajectory that matters most, but the uncovering of unambiguous features of the underlying dynamics of the system that produces it. The search for a model of a system differential invariant makes most sense as it contains all the information about the constants of motion. While initial conditions or even ‘states’ then seem like nuisance parameters, a model for the sought-after invariant emerges as an integral kernel. The ease of classical identification and Kalman state filtering is then traded for the hurdles of estimating the parameters of the kernels at the cost of the necessity to process large data sets. The gain is, however, that classical filtering is no longer necessary because the trajectory of interest together with all its derivatives (that might be thought to represent the states of some ‘canonical system realization’) are much better reconstructed than filtered.

It is believed that such way of thinking can inspire creation of ever faster and more accurate nonlinear state estimators and predictors that do not have to rely on a nonlinear model to deliver a Taylor series approximation.

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A Proof of Theorems 1 & 2

Multiplying equation (3) by the term \((\xi - a)^n\), yields
\[
(\xi - a)^n y^{(n)} + a_{n-1}(\xi - a)^{n-1} y + \cdots + a_1(\xi - a)^1 y + a_0(\xi - a)^0 y = 0
\]
\[(112)\]
This will be integrated multiple times on the interval \([a, a + \tau]\).

Multiplying equation (3) by the term \((b - \zeta)^n\), yields
\[
(b - \zeta)^n y^{(n)} + a_{n-1}(b - \zeta)^{n-1} y + \cdots + a_1(b - \zeta)^1 y + a_0(b - \zeta)^0 y = 0
\]
\[(113)\]
This will be integrated multiple times on the interval \([b - \sigma, b]\).

Integration by parts is used whenever it allows to lower the degree of the derivatives appearing under the integrals and the result is then simplified algebraically before proceeding to the next integration step.

Integration of the general term \((\xi - a)^n y^{(m)}\), (where \(n \geq m\)) over the interval \([a, a + \tau]\) yields the following expression:
\[
\int_a^{a+\tau} (\xi - a)^n y^{(m)}(\xi) d\xi = \sum_{i=0}^{m-1} (-1)^i \frac{n!}{(n-i)!} \tau^{n-i} y^{(m-i-1)}(a + \tau)
\]
\[
+ (-1)^m \frac{n!}{(n-m)!} \int_a^{a+\tau} (\xi - a)^n y(\xi) d\xi
\]
(See Theorem 3)

Kernel derivation for the output function \(y\)

An \(n\)-time integration of the general term \((\xi - a)^n y^{(m)}\) over the interval \([a, a + \tau]\) yields the following expressions:

For \(n = m\),
\[
\int_a^{(n)} (\xi - a)^n y^{(m)}(\xi) d\xi \cdots d\xi^{n-1} = \tau^n y + \sum_{j=1}^{n} (-1)^j \binom{n}{j} \frac{n!}{(n-j)!} \int_a^{(j)} (\xi - a)^n y(\xi) d\xi \cdots d\xi^{n-1}
\]

For \(n > m\),
\[
\int_a^{(n)} (\xi - a)^n y^{(m)}(\xi) d\xi \cdots d\xi^{n-1} = \sum_{j=0}^{m} (-1)^j \binom{m}{j} \frac{n!}{(n-j)!} \int_a^{(n-m+j)} (\xi - a)^n y(\xi) d\xi \cdots d\xi^{n-1}
\]
\( n \)-times integration of equation (112) on the interval \([a, a + \tau]\) gives

\[
\tau^n y + \sum_{j=1}^{n} (-1)^j \binom{n}{j} \frac{n!}{(n-j)!} \int^{(j)} (\xi - a)^{n-j} y(\xi) d\xi \ldots d\xi''
\]

\[
+ \sum_{i=0}^{n-1} a_i P_y(n, i) + \sum_{i=0}^{n-1} b_i P_u(n, i) = 0
\]

where

\[
P_y(n, i) = \sum_{j=0}^{i} (-1)^j \binom{i}{j} \frac{n!}{(n-j)!} \int^{(n-i+j)} (\xi - a)^{n-j} y(\xi) d\xi \ldots d\xi''
\]

\[
P_u(n, i) = \sum_{j=0}^{i} (-1)^j \binom{i}{j} \frac{n!}{(n-j)!} \int^{(n-i+j)} (\xi - a)^{n-j} u(\xi) d\xi \ldots d\xi''
\]

Applying the Cauchy formula for repeated integrals, while setting \( \tau + a = t \),

\[
(t - a)^n y + \sum_{j=1}^{n} (-1)^j \binom{n}{j} \frac{n!}{(n-j)!} \int^{t} (t - \xi)^{j-1} (\xi - a)^{n-j} y(\xi) d\xi
\]

\[
+ \sum_{i=0}^{n-1} a_i P_y(n, i) + \sum_{i=0}^{n-1} b_i P_u(n, i) = 0
\]

where

\[
P_y(n, i) = \sum_{j=0}^{i} (-1)^j \binom{i}{j} \frac{n!}{(n-j)!} \int^{t} (t - \xi)^{n-i+j-1} (\xi - a)^{n-j} y(\xi) d\xi
\]

\[
P_u(n, i) = \sum_{j=0}^{i} (-1)^j \binom{i}{j} \frac{n!}{(n-j)!} \int^{t} (t - \xi)^{n-i+j-1} (\xi - a)^{n-j} u(\xi) d\xi
\]

Swapping \( \int \) and \( \sum \) yields the forward kernel after some algebraic manipulation.

Forward kernel for output \( y \)

\[
y(t) = \frac{1}{(t-a)^n} \left[ \int_{a}^{t} K_{F,y}(n, t, \tau) y(\tau) d\tau + \int_{a}^{t} K_{F,u}(n, t, \tau) u(\tau) d\tau \right] \quad (114)
\]

where

\[
K_{F,y}(n, t, \tau) = \sum_{j=1}^{n} (-1)^{j+1} \binom{n}{j} \frac{n!}{(n-j)!} (t - \tau)^{j-1} (\tau - a)^{n-j}
\]
\[
+ \sum_{i=0}^{n-1} a_i \sum_{j=0}^{i} (-1)^{i+1} \binom{i}{j} \frac{n!}{(n-j)! (n-i+j-1)!} (t-\tau)^{n-i+j-1} (\tau-a)^{n-j}
\]

\[
K_{F,u}(n, t, \tau) = \sum_{i=0}^{n-1} b_i \sum_{j=0}^{i} (-1)^{i+1} \binom{i}{j} \frac{n!}{(n-j)! (n-i+j-1)!} (t-\tau)^{n-i+j-1} (\tau-a)^{n-j}
\]

The backward kernel is obtained similarly.

**Backward kernel for output \( y \)**

\[
y(t) = \frac{1}{(b-t)^n} \left[ \int_t^b K_{B,y}(n, t, \tau) y(\tau) d\tau + \int_t^b K_{B,u}(n, t, \tau) u(\tau) d\tau \right] \quad (115)
\]

where

\[
K_{B,y}(n, t, \tau) = \sum_{j=1}^{n} \binom{n}{j} \frac{n!}{(n-j)! (j-1)!} (t-\tau)^{j-1} (b-\tau)^{n-j}
\]

\[
+ \sum_{i=0}^{n-1} a_i \sum_{j=0}^{i} \binom{i}{j} \frac{n!}{(n-j)! (n-i+j-1)!} (t-\tau)^{n-i+j-1} (b-\tau)^{n-j}
\]

\[
K_{B,u}(n, t, \tau) = \sum_{i=0}^{n-1} b_i \sum_{j=0}^{i} \binom{i}{j} \frac{n!}{(n-j)! (n-i+j-1)!} (t-\tau)^{n-i+j-1} (b-\tau)^{n-j}
\]

Adding equations (114) and (115), yields

\[
y(t) = \frac{1}{(t-a)^n + (b-t)^n} \left[ \int_t^b K_{DS,y}(n, t, \tau) y(\tau) d\tau + \int_t^b K_{DS,u}(n, t, \tau) u(\tau) d\tau \right]
\]

where

\[
K_{DS,y}(n, t, \tau) \triangleq \begin{cases} 
K_{F,y}(n, t, \tau), & \text{for } \tau \leq t \\
K_{B,y}(n, t, \tau), & \text{for } \tau > t
\end{cases}
\]

\[
K_{DS,u}(n, t, \tau) \triangleq \begin{cases} 
K_{F,u}(n, t, \tau), & \text{for } \tau \leq t \\
K_{B,u}(n, t, \tau), & \text{for } \tau > t
\end{cases}
\]

**Kernels for the derivatives \( y^{(k)} \)**

To get the expression for the kernel for \( y^{(k)} \), the number of integrations to be performed is \( (n-k) \) times. They can also be calculated by direct differentiation of \( K_{F,y}, K_{B,y} \).
B  Theorem 3

Theorem 3  Integration of the general term \((\xi - a)^n y^{(m)}\), (where \(n \geq m\)) over the interval \([a, a + \tau]\) yields the following expression:

\[
\int_a^{a+\tau} (\xi - a)^n y^{(m)}(\xi) d\xi = \sum_{i=0}^{m-1} (-1)^i \frac{n!}{(n-i)!} \tau^{n-i} y^{(m-i-1)}(a + \tau) \\
+ (-1)^m \frac{n!}{(n-m)!} \int_a^{a+\tau} (\xi - a)^{n-m} y(\xi) d\xi 
\]

Proof by induction: Integration by parts is used whenever it allows to lower the degree of the derivatives appearing under the integrals and the result is then simplified algebraically before proceeding to the next integration.

Let us suppose equation 116 is true. Then,

\[
\int_a^{a+\tau} (\xi - a)^{n+1} y^{(m)}(\xi) d\xi \\
= (\xi - a)^{n+1} y^{(m-1)}(\xi) |_{a}^{a+\tau} - (n + 1) \int_a^{a+\tau} (\xi - a)^n y^{(m-1)}(\xi) d\xi \\
\quad \text{[integration by parts]} \\
= \tau^{n+1} y^{(m-1)}(a + \tau) - (n + 1) \left[ \sum_{i=0}^{m-2} (-1)^i \frac{n!}{(n-i)!} \tau^{n-i} y^{(m-i-2)}(a + \tau) \\
+ (-1)^{m-1} \frac{n!}{(n-m+1)!} \int_a^{a+\tau} (\xi - a)^{n-m+1} y(\xi) d\xi \right] \quad \text{[by equation 116]} \\
= \tau^{n+1} y^{(m-1)}(a + \tau) - \sum_{i=0}^{m-2} (-1)^i \frac{(n+1)!}{(n-i)!} \tau^{n-i} y^{(m-i-2)}(a + \tau) \\
+ (-1)^m \frac{(n+1)!}{(n-m+1)!} \int_a^{a+\tau} (\xi - a)^{n-m+1} y(\xi) d\xi \\
= \tau^{n+1} y^{(m-1)}(a + \tau) + \sum_{j=1}^{m-1} (-1)^j \frac{(n+1)!}{(n-j+1)!} \tau^{n-j+1} y^{(m-j-1)}(a + \tau) \\
+ (-1)^m \frac{(n+1)!}{(n-m+1)!} \int_a^{a+\tau} (\xi - a)^{n-m+1} y(\xi) d\xi \\
\quad \text{[Letting } j = i + 1] \\
= \sum_{j=0}^{m-1} (-1)^j \frac{(n+1)!}{(n+1-j)!} \tau^{n+1-j} y^{(m-j-1)}(a + \tau) \\
+ (-1)^m \frac{(n+1)!}{(n+1-m)!} \int_a^{a+\tau} (\xi - a)^{n+1-m} y(\xi) d\xi 
\]
It can be seen that equation (117) can also be obtained by replacing \( n \) with \( (n + 1) \) in equation (116).

Now, for \( n = 1, m = 1 \),

\[
\int_a^{a+\tau} (\xi - a)y^{(1)}(\xi)d\xi = (\xi - a)y(\xi)|_a^{a+\tau} - \int_a^{a+\tau} y(\xi)d\xi = \tau y(a+\tau) - \int_a^{a+\tau} y(\xi)d\xi
\]

For \( n = 2, m = 1 \),

\[
\int_a^{a+\tau} (\xi - a)^2y^{(1)}(\xi)d\xi = (\xi - a)^2y(\xi)|_a^{a+\tau} - 2\int_a^{a+\tau} (\xi - a)y(\xi)d\xi = \tau^2 y(a+\tau) - 2\int_a^{a+\tau} (\xi - a)y(\xi)d\xi
\]

Thus, equation (116) is true for \( n \geq 1 \) (when \( n \geq m \)).

C Kernels for 4th order homogeneous LTI system

\[K_{F,y}(4, t, \tau) = 16(\tau - a)^3 - a_3(\tau - a)^4 + (t - \tau)\left[-72(\tau - a)^2 + 12a_3(\tau - a)^3 - a_2(\tau - a)^4\right] + \frac{(t - \tau)^2}{2}\left[96(\tau - a) - 36a_3(\tau - a)^2 + 8a_2(\tau - a)^3 - a_1(\tau - a)^4\right] + \frac{(t - \tau)^3}{6}\left[-24 + 24a_3(\tau - a) - 12a_2(\tau - a)^2 + 4a_1(\tau - a)^3 - a_0(\tau - a)^4\right]\]

\[K_{B,y}(4, t, \tau) = 16(b - \tau)^3 + a_3(b - \tau)^4 + (t - \tau)\left[72(b - \tau)^2 + 12a_3(b - \tau)^3 + a_2(b - \tau)^4\right] + \frac{(t - \tau)^2}{2}\left[96(b - \tau) + 36a_3(b - \tau)^2 + 8a_2(b - \tau)^3 + a_1(b - \tau)^4\right] + \frac{(t - \tau)^3}{6}\left[24 + 24a_3(b - \tau) + 12a_2(b - \tau)^2 + 4a_1(b - \tau)^3 + a_0(b - \tau)^4\right]\]

The derivative kernels for the reconstruction of \( y_E^{(i)}, i = 1, 2, 3 \) are omitted as they can be calculated by direct differentiation of \( K_{F,y}, K_{B,y} \).

D A feasible recursive GLS algorithm

Recalling equations (41) and (87):
\[
\hat{a}_k = \arg \min_a \left( \sum_{i=1}^{k} (Q_i - P_i \hat{a})^T S_i (Q_i - P_i \hat{a}) \right)
\] (118)

Defining \( M_{k+1} = \sum_{i=0}^{k+1} P_i^T S_i P_i \) and \( R_{k+1} = M_{k+1}^{-1} \), the feasible recursive GLS algorithm comprises two update equations:

\[
\begin{align*}
\hat{a}_{k+1} &= \hat{a}_k + R_{k+1} P_k^T (Q_{k+1} - P_{k+1} \hat{a}_k) \\
R_{k+1} &= R_k - R_k P_k^T (S_{k+1}^{-1} + P_{k+1} R_k P_k^T)^{-1} P_{k+1} R_k
\end{align*}
\] (119) (120)

**Initialization of the GLS**

The initial estimate of \( \sigma^2 \) is calculated as the *empirical* variance of \(( y_M - y_E )\) where \( y_E \) is the estimated output corresponding to the parameter values obtained in iteration \( k = 0 \). This is updated at each consecutive iteration by the same empirical method.