

Efficient identification of oblique Volterra systems

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Abstract. A computationally efficient method is described for estimating first-order and associated higher-order kernels of general multi-input Volterra systems expressed in the oblique (nonsymmetric) form. A first-order kernel characterizes how a system responds to isolated inputs (i.e., an isolated input-output transformation), and the oblique form interprets a higher-order kernel as modifying an input-output transformation for one specific (target) input channel in the context of other inputs. Context is quantified as products of the target input channel with one or more input channels lagged with respect to the target. The full system is Fourier transformed, and orthonormal basis functions are stipulated for inter-channel lags in the frequency domain. The system then reduces to a linearized form. Basis factors associated with the input products (“q-factors”) are calculated for each experimental realization, and then basis coefficients associated with unknown kernels (“a-coefficients”) are found via complex singular value decomposition (SVD) at each frequency, across all realizations. SVD permits singular situations to be diagnosed and treated. Finally, kernels are reconstructed in the time domain via inverse Fourier transformation. New applications are envisioned in systems neuroscience, and in cognitive neurophysiology using continuous sensorimotor tasks.

Keywords: Nonlinear; Frequency Domain; Robust Estimation; Continuous Behavioral Paradigms; Neurophysiological Data

1. Introduction

Cognitive-behavioral experiments with neurophysiological data (such as EEG or MEG) typically use event-related paradigms, which are well suited for laboratory controls, yet otherwise are highly simplified compared with life outside the lab. In particular, daily life often requires monitoring of *continuous* variables in real time concurrently with graded behavioral adjustments (e.g., sensorimotor tracking) in contrast with—or in addition to—discrete stimulus detection and ballistic response production. It is unclear how to analyze neurophysiological data acquired with continuous paradigms, and whether event-related analysis might be generalized for integration with continuous analysis.

A companion paper [Pflieger, 2011] presents a theory of event-related Volterra (ERV) modeling, a nonlinear generalization of Hansen decomposition [Hansen, 1983] which, in turn, generalizes the ubiquitous method of event-related averaging. Here we show that computationally efficient ERV model estimation, which employs basis functions in the frequency domain, can be extended to handle general Volterra systems with continuous input functions.

The Volterra-Wiener approach to system identification [Schetzen, 1980] originated with Volterra [1930] and Wiener [1958] as general expansions for input-output transfer functions, originally for one input time series and one output time series, and later generalized to the multi-input case [Marmarelis & Naka, 1974]. The multi-output case is handled simply by separate treatment for each output function. Analogous to Taylor series expansions, the main idea is to approximate an arbitrary transfer function by truncating an expansion at a finite order. A first-order *kernel* is the familiar impulse response function of linear system theory; it is convolved with an input time series to produce an output time series. By generalizing convolution to include two or more time lags, the same relationship holds for second- and higher-order kernels (see Eq. (1)). In neuroscience, various kernel estimation methods have been applied in somatosensory [Sclabassi et al., 1985], visual [Pinter & Nabet, 1992], auditory [Eggermont, 1993], CNS network analysis [Sclabassi et al., 1988][Song et al., 2009], and functional neuroimaging [Friston et al., 1998] studies.

Because Wiener expansions are optimized for specially randomized inputs (such as white noise), which are not generally useful in cognitive-behavioral experiments, this paper focuses on Volterra expansions. Section 2 introduces inter-lag intervals (ILIs) and inter-lagged multi-products for an *oblique* reinterpretation of the standard symmetric Volterra expansion. This sets up Section 3’s frequency domain approach using ILI basis functions. Section 4 describes how to calculate the input-related factors associated with ILI basis functions for each term of the Volterra expansion. These “q-factors” are applied in Section 5 to obtain the kernel-related coefficients of the ILI basis functions in the context of a singularity analysis, which is needed to insure adequate experimental design and robust

estimation. After all kernels have been expanded in the frequency domain, they are reconstructed in the time domain, where their interpretation may shed light on the observed system behavior.

2. Oblique Volterra systems

On each realization (e.g., trial) j , a Volterra system with L inputs (e.g., sensory or motor task variables) $x_{j1}(), \dots, x_{jL}()$ generates an output time series (e.g., data on a neurophysiological channel) $y_j()$ via a functional series expansion, as follows:

$$y_j(t) \approx \varepsilon_j(t) + \sum_{i_1=1}^L \left(\int h_{i_1}^{(1)}(\tau_1) x_{ji_1}(t - \tau_1) d\tau_1 + \sum_{i_2=1}^L \left(\iint h_{i_1 i_2}^{(2)}(\tau_1, \tau_2) x_{ji_1}(t - \tau_1) x_{ji_2}(t - \tau_2) d\tau_1 d\tau_2 + \sum_{i_3=1}^L \left(\iiint h_{i_1 i_2 i_3}^{(3)}(\tau_1, \tau_2, \tau_3) x_{ji_1}(t - \tau_1) x_{ji_2}(t - \tau_2) x_{ji_3}(t - \tau_3) d\tau_1 d\tau_2 d\tau_3 + \dots \right) \right) \right) \quad (1)$$

where $\varepsilon_j()$ is random error, and all integrals are from $-\infty$ to ∞ . The Volterra system is characterized by its *kernels*, which are invariant across realizations: $h_{i_1}^{(1)}()$ is a first-order kernel (i.e., impulse response function); $h_{i_1 i_2}^{(2)}(,)$ is a second-order kernel; $h_{i_1 i_2 i_3}^{(3)}(,,)$ is a third-order kernel; and so on. The standard form of Eq. (1) treats all lags $\tau_1, \tau_2, \dots$ symmetrically. In the equivalent *oblique form*, the first lag τ_1 is provided a special status with respect to the time variable t , and the other lags are parameterized relative to τ_1 as *inter-lag intervals* $\sigma_{12} \equiv \tau_1 - \tau_2, \sigma_{13} \equiv \tau_1 - \tau_3, \dots$:

$$y_j(t) \approx \varepsilon_j(t) + \sum_{i_1=1}^L \left(\int h_{i_1}^{(1)}(\tau_1) x_{ji_1}(t - \tau_1) d\tau_1 + \sum_{i_2=1}^L \left(\iint \underline{h}_{i_1 i_2}^{(2)}[\sigma_{12}](\tau_1) x_{ji_1}(t - \tau_1) x_{ji_2}(t - \tau_1 - \sigma_{12}) d\tau_1 d\sigma_{12} + \sum_{i_3=1}^L \left(\iiint \underline{h}_{i_1 i_2 i_3}^{(3)}[\sigma_{12}, \sigma_{13}](\tau_1) x_{ji_1}(t - \tau_1) x_{ji_2}(t - \tau_1 - \sigma_{12}) x_{ji_3}(t - \tau_1 - \sigma_{12} - \sigma_{13}) d\tau_1 d\sigma_{12} d\sigma_{13} + \dots \right) \right) \right) \quad (2)$$

Underscores indicate kernels in oblique form. *Inter-lagged multi-products* are defined as

$$x_{ji_2}[\sigma_{12}](t) \equiv x_{ji_1}(t) x_{ji_2}(t + \sigma_{12}), \quad (3)$$

$$x_{ji_2 i_3}[\sigma_{12}, \sigma_{13}](t) \equiv x_{ji_1}(t) x_{ji_2}(t + \sigma_{12}) x_{ji_3}(t + \sigma_{12} + \sigma_{13}), \quad (4)$$

and in general

$$x_{ji_2 \dots i_m}[\sigma_{12}, \dots, \sigma_{1m}](t) \equiv x_{ji_1}(t) x_{ji_2}(t + \sigma_{12}) \dots x_{ji_m}(t + \sigma_{12} + \dots + \sigma_{1m}). \quad (5)$$

The oblique form interprets each kernel, of any order, as an inter-lag interval (ILI) *parameterized transient waveform*: a first-order kernel is a transient waveform without parameters; a second-order kernel is a transient with one ILI parameter; a third-order kernel is a transient with two ILIs; and so on. A key feature of the oblique form is that *all kernels with the same target index i_1 also share a common time base (τ_1)*. Kernels and their associated inter-lagged multi-products share exactly the same ILI parameters. Finally, like the kernels, inter-lagged multi-products with the same target index i_1 also share a common time base ($t - \tau_1$).

Thus, a natural interpretation for the oblique form is that higher-order terms *modify* their associated first- and lower-order terms. That is, the primary system phenomenon associated with input variable $x_{j i_1}()$ is a *transient component* comprising all terms with the same i_1 index. In yet other words, a kernel's target index specifies a *primary transient* associated with an input variable, and the remaining indices specify *secondary modulations* via lags associated with the same or other input variables.

3. Frequency domain formulation using ILI basis functions

The Fourier transform of Eq. (2) is

$$Y_j(f) \approx E_j(f) + \sum_{i_1=1}^L \left(H_{i_1}^{(1)}(f) X_{j i_1}(f) + \sum_{i_2=1}^L \left(\int H_{i_1 i_2}^{(2)}[\sigma_{12}](f) X_{j i_1 i_2}[\sigma_{12}](f) d\sigma_{12} + \sum_{i_3=1}^L \left(\int \int H_{i_1 i_2 i_3}^{(3)}[\sigma_{12}, \sigma_{13}](f) X_{j i_1 i_2 i_3}[\sigma_{12}, \sigma_{13}](f) d\sigma_{12} d\sigma_{13} + \dots \right) \right) \right) \quad (6)$$

where uppercase denotes the Fourier transform of a corresponding lowercase time series. The τ_1 lags integrated out when waveform convolutions converted to multiplications in the frequency domain.

Next, a set of *orthonormal basis functions* is stipulated for each ILI integration parameter σ_{1m} :

$$b_1^{(i_{1m})}(\sigma_{1m}), b_2^{(i_{1m})}(\sigma_{1m}), \dots, b_{B_{i_{1m}}}^{(i_{1m})}(\sigma_{1m}) \quad (7)$$

so that the order > 1 kernels and multi-lag products can be approximated as

$$H_{i_1 i_2 \dots i_m}^{(m)}[\sigma_{12}, \dots, \sigma_{1m}](f) \approx \sum_{k_{12}=1}^{B_{i_{12}}} \dots \sum_{k_{1m}=1}^{B_{i_{1m}}} a_{k_{12} \dots k_{1m}}^{(i_{12} \dots i_m)}(f) b_{k_{12}}^{(i_{12})}(\sigma_{12}) \dots b_{k_{1m}}^{(i_{1m})}(\sigma_{1m}) \quad (8)$$

and

$$X_{j i_1 i_2 \dots i_m}[\sigma_{12}, \dots, \sigma_{1m}](f) \approx \sum_{k_{12}=1}^{B_{i_{12}}} \dots \sum_{k_{1m}=1}^{B_{i_{1m}}} q_{k_{12} \dots k_{1m}}^{(j i_1 i_2 \dots i_m)}(f) b_{k_{12}}^{(i_{12})}(\sigma_{12}) \dots b_{k_{1m}}^{(i_{1m})}(\sigma_{1m}). \quad (9)$$

Consequently, a third-order term (as a prototypical case) expands, and then reduces, as follows:

$$\begin{aligned} \int \int H_{i_1 i_2 i_3}^{(3)}[\sigma_{12}, \sigma_{13}](f) X_{j i_1 i_2 i_3}[\sigma_{12}, \sigma_{13}](f) d\sigma_{12} d\sigma_{13} \approx \\ \int \int \left(\sum_{k_{12}=1}^{B_{i_{12}}} \sum_{k_{13}=1}^{B_{i_{13}}} a_{k_{12} k_{13}}^{(i_{12} i_{13})}(f) b_{k_{12}}^{(i_{12})}(\sigma_{12}) b_{k_{13}}^{(i_{13})}(\sigma_{13}) \right) \left(\sum_{k_{12}=1}^{B_{i_{12}}} \sum_{k_{13}=1}^{B_{i_{13}}} q_{k_{12} k_{13}}^{(j i_1 i_2 i_3)}(f) b_{k_{12}}^{(i_{12})}(\sigma_{12}) b_{k_{13}}^{(i_{13})}(\sigma_{13}) \right) d\sigma_{12} d\sigma_{13} = \\ \sum_{k_{12}=1}^{B_{i_{12}}} \sum_{k_{13}=1}^{B_{i_{13}}} \sum_{k_{12}^{(H)}=1}^{B_{i_{12}^{(H)}}} \sum_{k_{13}^{(H)}=1}^{B_{i_{13}^{(H)}}} a_{k_{12}^{(H)} k_{13}^{(H)}}^{(i_{12} i_{13})}(f) q_{k_{12}^{(H)} k_{13}^{(H)}}^{(j i_1 i_2 i_3)}(f) \left(\int b_{k_{12}^{(H)}}^{(i_{12})}(\sigma_{12}) b_{k_{12}^{(H)}}^{(i_{12})}(\sigma_{12}) d\sigma_{12} \right) \left(\int b_{k_{13}^{(H)}}^{(i_{13})}(\sigma_{13}) b_{k_{13}^{(H)}}^{(i_{13})}(\sigma_{13}) d\sigma_{13} \right) = \\ \sum_{k_{12}=1}^{B_{i_{12}}} \sum_{k_{13}=1}^{B_{i_{13}}} q_{k_{12} k_{13}}^{(j i_1 i_2 i_3)}(f) a_{k_{12} k_{13}}^{(i_{12} i_{13})}(f) \end{aligned} \quad (10)$$

where the final reduction—with both ILI parameters having integrated out—results from orthonormality of the stipulated set of basis functions. The reduction of Eq. (10) clearly generalizes, so that an order M oblique Volterra system in the frequency domain has the linearized form

$$Y_j(f) = E_j(f) + \sum_{i_1=1}^L \beta_{i_1} q^{(j i_1)}(f) a^{(i_1)}(f) + \sum_{m=2}^L \sum_{i_1=1}^L \dots \sum_{i_m=1}^L \beta_{i_1 \dots i_m} \sum_{k_{12}=1}^{B_{i_{12}}} \dots \sum_{k_{1m}=1}^{B_{i_{1m}}} q_{k_{12} \dots k_{1m}}^{(j i_1 \dots i_m)}(f) a_{k_{12} \dots k_{1m}}^{(i_1 \dots i_m)}(f) \quad (11)$$

where *selection booleans* $\beta_{\bullet}$ have been inserted to specify (from the full model) whether a partial model shall include ($\beta_{\bullet} = 1$) or exclude ($\beta_{\bullet} = 0$) a particular kernel's term. The unknown a-coefficients may be obtained using linear methods; then the kernels are reconstructed in the frequency domain via Eq. (8). Before this can proceed, however, the input-driven q-factors must be calculated.

4. Calculation of q-factors

Equation (9) is the foundation for determining the q-factors associated with a given higher-order term. For each realization and each frequency, there are $B = B_{i_{12}} \dots B_{i_{1m}}$ such factors; whereas the

input data consist of $\mathbf{S}$ combinations of ILIs for the multi-lag products, which come from Eq. (5). In theory, the integral for each ILI σ is unbounded; but in experimental practice, bounds from $\sigma^{\min}$ to $\sigma^{\max}$ must be specified, and a finite number of ILIs are sampled within this range; so that $\mathbf{S} = \mathbf{S}_{i_1 i_2} \cdots \mathbf{S}_{i_1 i_m}$ is the product of these numbers across all ILI parameters. Because the basis functions are a means of approximation, $B_{i_1 i_k} < S_{i_1 i_k}$, and typically $B \ll S$. Thus, a complex linear system with more equations than unknown q-factors can be set up from the following definitions:

$$\mathbf{P}_{i_1 \cdots i_m} \equiv \begin{bmatrix} b_1^{(i_1 i_2)}(\sigma_{12}^{(1)}) \cdots b_1^{(i_1 i_m)}(\sigma_{1m}^{(1)}) & \cdots & b_{B_{i_1 i_2}}^{(i_1 i_2)}(\sigma_{12}^{(1)}) \cdots b_{B_{i_1 i_m}}^{(i_1 i_m)}(\sigma_{1m}^{(1)}) \\ \vdots & \ddots & \vdots \\ b_1^{(i_1 i_2)}(\sigma_{12}^{(S_{i_1 i_2})}) \cdots b_1^{(i_1 i_m)}(\sigma_{1m}^{(S_{i_1 i_m})}) & \cdots & b_{B_{i_1 i_2}}^{(i_1 i_2)}(\sigma_{12}^{(S_{i_1 i_2})}) \cdots b_{B_{i_1 i_m}}^{(i_1 i_m)}(\sigma_{1m}^{(S_{i_1 i_m})}) \end{bmatrix} \quad (12)$$

$$\mathbf{q}_{j i_1 \cdots i_m}(f) \equiv \begin{bmatrix} q_{1 \cdots 1}^{(j i_1 \cdots i_m)}(f) \\ \vdots \\ q_{B_{i_1 i_2} \cdots B_{i_1 i_m}}^{(j i_1 \cdots i_m)}(f) \end{bmatrix} \quad \mathbf{X}_{j i_1 \cdots i_m}(f) \equiv \begin{bmatrix} X_{j i_1 \cdots i_m}[\sigma_{12}^{(1)}, \cdots, \sigma_{1m}^{(1)}](f) \\ \vdots \\ X_{j i_1 \cdots i_m}[\sigma_{12}^{(S_{i_1 i_2})}, \cdots, \sigma_{1m}^{(S_{i_1 i_m})}](f) \end{bmatrix}$$

Namely,

$$\mathbf{P}_{i_1 \cdots i_m} \mathbf{q}_{j i_1 \cdots i_m}(f) = \mathbf{X}_{j i_1 \cdots i_m}(f) \quad (13)$$

Consequently, the q-factors are calculated as follows:

$$\mathbf{q}_{j i_1 \cdots i_m}(f) = \mathbf{P}_{i_1 \cdots i_m}^+ \mathbf{X}_{j i_1 \cdots i_m}(f) = \left(\mathbf{P}_{i_1 \cdots i_m}^* \mathbf{P}_{i_1 \cdots i_m} \right)^{-1} \mathbf{P}_{i_1 \cdots i_m}^* \mathbf{X}_{j i_1 \cdots i_m}(f) \quad (14)$$

Invertibility of the $B \times B$ matrix $\mathbf{P}_{i_1 \cdots i_m}^* \mathbf{P}_{i_1 \cdots i_m}$ is a requirement to be met by suitable selection of ILI basis functions and ILI samples of multi-lag products. Note that the $B \times S$ pseudoinverse matrix $\mathbf{P}_{i_1 \cdots i_m}^+$ correlated with each kernel can be precalculated *once* for all realizations and all frequencies.

5. Solution via complex singular value decomposition (SVD)

For J realizations, Eq. (11) may be written in matrix form as

$$\mathbf{Q}(f) \mathbf{a}(f) \approx \mathbf{Y}(f) \quad (15)$$

where

$$\mathbf{Q}(f) \equiv \begin{bmatrix} q^{(11)}(f) & \cdots & q_{B_{LL} \cdots B_{LL}}^{(1L \cdots L)}(f) \\ \vdots & \ddots & \vdots \\ q^{(J1)}(f) & \cdots & q_{B_{LL} \cdots B_{LL}}^{(JL \cdots L)}(f) \end{bmatrix} \quad \mathbf{a}(f) \equiv \begin{bmatrix} a^{(1)}(f) \\ \vdots \\ a_{B_L \cdots B_L}^{(L \cdots L)}(f) \end{bmatrix} \quad \mathbf{Y}(f) \equiv \begin{bmatrix} Y_1(f) \\ \vdots \\ Y_J(f) \end{bmatrix} \quad (16)$$

and it is understood that only the boolean-selected terms have been included. The solution via complex singular value decomposition (SVD) [Golub & Van Loan, 1996][Press et al., 1988] is

$$\begin{aligned} \text{svd}(\mathbf{Q}(f)) &= \mathbf{U}(f) \mathbf{W}(f) \mathbf{V}(f)^* \\ \mathbf{a}(f) &\approx \mathbf{V}(f) \mathbf{W}(f)^+ \mathbf{U}(f)^* \mathbf{Y}(f) \end{aligned} \quad (17)$$

where $\mathbf{W}(f)$ is a diagonal matrix of non-negative real singular values, and $\mathbf{W}(f)^+$ is obtained by forming reciprocal singular values unless they are close to zero, in which case the researcher must decide whether to regularize the solution by setting the corresponding reciprocals to zero, or to modify the experiment. In particular, singular values close to zero may indicate that the experiment is inadequate to identify the selected kernels: It may have too few realizations (trials), or the experimental input variables may have been insufficiently randomized across realizations. Per Section 4, note that the $\mathbf{Q}$ -matrix is derived from the input time series. To the extent that these are planned, experimental adequacy may be assessed before acquiring the output data.

To complete the solution, a-coefficients at each frequency are used in Eq. (8) to reconstruct the kernels, which ultimately are inverse Fourier transformed to the time domain.

If the error process spectral density $|E_j(f)|$ is available, it may be used to whiten $\mathbf{Y}(f)$ and $\mathbf{Q}(f)$ by simple division, in which case the whitened $\bar{\mathbf{Y}}(f)$ and $\bar{\mathbf{Q}}(f)$ may be substituted in Eq. (17). Unless estimates of the error process can be made for each experimental realization, the whitened and unwhitened solutions are algebraically equivalent.

6. Discussion

Theoretical results of this paper demonstrate that an efficient frequency domain solution method for discrete event-related Volterra (ERV) models [Pflieger, 2011] can be extended to general Volterra models. The oblique form using inter-event intervals (IEIs) in the ERV case was generalized here to an oblique form using inter-lag intervals (ILIs) with inter-lag multi-products of the input time series. The oblique form does not restrict the generality of a Volterra system, but is an alternative interpretation, equivalent to the standard symmetric form. Final solutions in both cases (this paper's Eq. (17), and Eq. (7) in [Pflieger, 2011]) share an identical form. The key difference is that the general method for calculating the Q-matrix via Eq. (14) requires considerably more machinery compared with simple recursive formulas for q-factors in the ERV case.

Although the general method is inefficient for the discrete event-related case, it can handle continuous input time series efficiently and robustly. In particular, one large system of equations in the time domain has been reduced to many smaller systems of complex linear equations in the frequency domain, where singularity analysis is performed for each inversion step to confirm adequate experimental design and repetitions. In addition, a singularity analysis may be performed in advance of acquiring the output data to facilitate experimental planning.

In addition to enabling efficient computation, the oblique form also facilitates *interpretation* of an identified higher-order kernel, which is associated with exactly one target input time series, and modifies its first-order kernel in the context of other input time series. The first-order kernel for an input time series characterizes how the system responds in isolation from other inputs (whether from other-indexed input channels, or at other times on the same-indexed channel). In the oblique interpretation, higher-order kernels convey the contextual effect of other inputs by adding to, or subtracting from, the first-order kernel. In other words, they transform input-output transformations.

Potentially, the method may be applied in various scientific domains that deal with multiple time series, including systems neuroscience at several levels of analysis. At the top level, applications are envisioned in the domain of cognitive-behavioral neurophysiology: brain signals and modulations related to continuous variables may be studied in contexts such as eye tracking, or robot-assisted sensorimotor training for stroke rehabilitation.

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