WORD SERIES FOR DYNAMICAL SYSTEMS

J. M. Sanz-Serna

Universidad Carlos III de Madrid

I: DEFINING WORD SERIES

A MOTIVATING EXAMPLE:

$$\frac{d}{dt}x = \sum_{a \in A} \lambda_a(t) f_a(x).$$

- A finite or infinite index set (alphabet).
- $f_a(x)$ vector field in D dimensions.
- $\lambda_a(t)$ scalar-valued function.

- Solution with $x(0) = x_0$ given by (cf Chen series)

$$x(t) = x_0 + \sum_{n=1}^{\infty} \sum_{a_1,\ldots,a_n \in A} \alpha_{a_1 \cdots a_n}(t) f_{a_1 \cdots a_n}(x_0),$$

with $\alpha_{a_1 \cdots a_n}(t)$ given by

$$\int_0^t dt_n \, \lambda_{a_n}(t_n) \int_0^{t_n} dt_{n-1} \, \lambda_{a_{n-1}}(t_{n-1}) \cdots \int_0^{t_2} dt_1 \, \lambda_{a_1}(t_1),$$

and, recursively,

$$f_{a_1 \cdots a_n}(x) = \partial_x f_{a_2 \cdots a_n}(x) \, f_{a_1}(x).$$

WORDS AND THEIR BASIS FUNCTIONS

- $\mathcal{W}$ denotes set of all letters from the alphabet A (including the empty word); $\mathcal{W}_n$ is the set of words with n letters.

- Associate with $w = a_1 \cdots a_n \in \mathcal{W}$ its word basis function $f_w(x) = f_{a_1 \cdots a_n}(x)$ (with $f_\emptyset(x) \equiv x$).

DEFINITION

• If $\delta \in \mathbb{C}^{\mathcal{W}}$ (ie δ maps words into scalars), the word series with coefficients δ is the formal series:

$$W_\delta(x) = \sum_{w \in \mathcal{W}} \delta_w f_w(x).$$

• Note that the notion of word series is relative to the f_a.

• For each t, the solution value $x(t)$ corresponds to the coefficients $\alpha_w(t)$ built above from the $\lambda_a(t)$.

WORD SERIES VS B-SERIES

- Each word series function is a linear combination of coloured elementary differentials (relative to the same f_a), eg

$$f_{cba}(x) = \partial_{xx} f_a(x)[f_b(x), f_c(x)] + \partial_x f_a(x)\, \partial_x f_b(x)\, f_c(x).$$

- Hence each word series may be rewritten as a (coloured) B-series.

SOME PARTICULAR CASES:

EXAMPLE I: A consists of a single letter a. For each n there is a single word $w = a \cdots a$ with n letters.

If furthermore $\lambda_a(t) \equiv 1$, $\alpha_w(t)$, $w \in \mathcal{W}_n$ is found to be $t^n/n!$. The word series $W_{\alpha(t)}(x_0)$ is the Taylor expansion in powers of t of the solution $x(t)$ of $(d/dt)x = f_a(x)$, $x(0) = x_0$. Runge-Kutta solutions may be expanded as B-series; the class of word series is too narrow to accommodate them.

EXAMPLE II: A consists of a two letters a, b. For each n there are 2^n words with n letters.

If furthermore $\lambda_a(t) \equiv 1$, $\lambda_b(t) \equiv 1$, $\alpha_w(t) = t^n/n!$ for $w \in \mathcal{W}_n$. The word series $W_{\alpha(t)}(x_0)$ is the Taylor expansion of $x(t)$, $(d/dt)x = f_a(x) + f_b(x)$, written in terms of f_a, f_b. Additive Runge-Kutta solutions may be expanded as B-series; the class of word series is too narrow to accommodate them.

EXAMPLE III: Fix $\omega > 0$. If $A = \mathbb{Z}$ and, for $k \in \mathbb{Z}$,

$$\lambda_k(t) = \exp(ik\omega t),$$

then $(d/dt)x = \sum_a \lambda_a(t) f_a(x)$ is a *non-autonomous* system $2\pi/\omega$-periodic in t with the right-hand side expanded in Fourier series.

Quasiperiodic systems may be similarly considered.

II: OPERATING WITH WORD SERIES

THE CONVOLUTION PRODUCT

- If $\delta, \delta' \in \mathbb{C}^{\mathcal{W}}$, their *convolution product* $\delta \star \delta' \in \mathbb{C}^{\mathcal{W}}$ is

$$(\delta \star \delta')_{a_1 \cdots a_n} = \delta_{\emptyset} \delta'_{a_1 \cdots a_n} + \sum_{j=1}^{n-1} \delta_{a_1 \cdots a_j} \delta'_{a_{j+1} \cdots a_n} + \delta_{a_1 \cdots a_n} \delta'_{\emptyset}$$

- Not commutative.

- Associative.

- Unit: $\mathbb{1} \in \mathbb{C}^{\mathcal{W}}$ with $\mathbb{1}_{\emptyset} = 1$ and $\mathbb{1}_{w} = 0$ for $w \neq \emptyset$.

THE GROUP $\mathcal{G}$

- Let $\sqcup\!\sqcup$ denote shuffle product of words.

- Let $\mathcal{G}$ be the set of those $\gamma \in \mathbb{C}^{\mathcal{W}}$ that satisfy the so-called *shuffle relations:* $\gamma_\emptyset = 1$ and, for each $w, w' \in \mathcal{W}$,

$$\gamma_w \gamma_{w'} = \sum_{j=1}^{N} \gamma_{w_j} \qquad \text{if} \qquad w \sqcup\!\sqcup w' = \sum_{j=1}^{N} w_j.$$

- $(\mathcal{G}, \star)$ is a noncommutative group. (Group of characters of shuffle Hopf algebra.)

• Important to keep in mind that for $\gamma \in \mathcal{G}$ the γ_w are not 'free' parameters.

• For $\gamma \in \mathcal{G}$, the series $W_\gamma(x)$ acts on the vector space of all word series by composition:

$$W_\delta\big(W_\gamma(x)\big) = W_{\gamma\star\delta}(x), \quad \delta \in \mathbb{C}^{\mathcal{W}}.$$

• For arbitrary $\lambda_a(t)$ and each fixed t, the coefficients $\alpha(t) \in \mathbb{C}^{\mathcal{W}}$ defined previously are an element of $\mathcal{G}$.

APPLICATION: SPLITTING

• Given $(d/dt)x = f_a(x) + f_b(x)$, $s, t \in \mathbb{R}$, the flows φ_s^a and φ_t^b of $(d/dt)x = f_a(x)$ and $(d/dt)x = f_b(x)$ correspond, as noted above, to elements of G.

• Hence, for each time-step h, the one-step map ψ_h of a splitting integrator will also correspond to an element of G. The coefficients are easily found by means of the operation $\star$.

CHANGING VARIABLES

• For $\gamma \in \mathcal{G}$, word series $W_\gamma(x)$ are equivariant with respect to arbitrary changes of variables $x = C(X)$:

$$W_\gamma(x) = W_\gamma(C(X)) = C(\widetilde{W}_\gamma(X)),$$

where the tilde means that in $\widetilde{W}_\gamma(X)$ the word basis functions are built from the vector fields $(\partial C(X))^{-1} f_a(C(X))$.

(Cf McLachlan, Modin, Munthe-Kaas, Verdier.)

THE LIE ALGEBRA $\mathfrak{g}$ OF THE GROUP $\mathcal{G}$:

- May also be described in terms of word series (details will not be given).

- Plays a role in analyzing splitting integrators (eg modified equations).

III: AVERAGING

THE AIM

- Given an oscillatory system

$$\frac{d}{dt}x = \epsilon f(x, \omega t),$$

where $\omega > 0$ and $f(x, \theta)$ is 2π-periodic in θ, find a change of variables $x = U(X, \theta; \epsilon)$ (2π-periodic in θ), such that the substitution $x(t) = U(X(t), \omega t; \epsilon)$ maps its solutions into solutions of

$$\frac{d}{dt}X = \epsilon \bar{F}(X; \epsilon).$$

(an autonomous system).

USUALLY . . .

• A sequence of changes of variables is performed in the system $(d/dt)x = \epsilon f(x, \omega t)$.

• The first change results in a system $(d/dt)x_1 = \epsilon F_1(x_1) + \epsilon^2 f_1(x_1, \omega t)$: the explicit dependence on t is brought down to $\mathcal{O}(\epsilon^2)$.

• Successive changes to get $\mathcal{O}(\epsilon^3)$, $\mathcal{O}(\epsilon^4)$, . . .

OUR PRESCRIPTION

- Write given system in the form (seen before):

$$\frac{d}{dt}x = \sum_{k\in\mathbb{Z}} \exp(ik\omega t)\epsilon f_k(x).$$

[Note this is of the form

$$\frac{d}{dt}x = W_{\beta(\omega t)}(x).$$

(relative to basis functions constructed from the vector fields $\epsilon f_k(x)$), where $\beta_k(\theta) = \exp(ik\theta)$ for one letter words.]

- We know that solution $x(t)$ is a word series $W_{\alpha(t)}(x(0))$.

- Analyze the structure of $W_{\alpha(t)}(x(0))$.

- We thus focus on solutions rather than on equations.

THE TECHNIQUE DELIVERS:

- An averaged differential system written as a word series

$$\frac{d}{dt}X = W_{\overline{\beta}}(X).$$

- The required change of variables

$$x = U(X, \theta; \epsilon) = W_{\kappa(\theta)}(X).$$

- The coefficients $\overline{\beta}$ and $\kappa(\theta)$ are universal (independent of f) and may be computed through simple recursions.

ANALYZING $W_{\alpha(t)}(x(0))$

Example: for the two letter word $k(-k)$, $k \neq 0$

$$\alpha_w(t) = \frac{it}{k\omega} + \frac{1 - \exp(ik\omega t)}{k^2\omega^2}.$$

KEY OBSERVATION

- For each word $w \in \mathcal{W}$ the coefficient $\alpha_w(t)$ is of the form $\gamma_w(t, \omega t)$, with $\gamma_w(t, \theta)$ a polynomial in t, $\exp(i\theta)$, $\exp(-i\theta)$.

- Hence the series $X(t) = W_{\gamma(t,0)}(x(0))$ interpolates at the stroboscopic times $m(2\pi)/\omega$, m integer, the (oscillatory) solution $x(t) = W_{\gamma(t,\omega t)}(x(0))$ and is not oscillatory.

- $X(t)$ candidate to solution of averaged system?

TRANSPORT EQUATION

- Since $\alpha(t)$ solves $(d/dt)x = W_{\beta(\omega t)}(x)$, we may write

$$\frac{d}{dt}\alpha(t) = \alpha(t) \star \beta(\omega t)$$

(recall $\star$ is compositon and note universality).

- If $\alpha(t) = \gamma(t, \omega t)$, then seek $\gamma(t, \theta)$ as solution of

$$\partial_t \gamma(t, \theta) + \omega \partial_\theta \gamma(t, \theta) = \gamma(t, \theta) * \beta(\theta).$$

- Initially $\gamma(0,0) = \mathbb{1}$.

- May prove that transport equation + initial condition + polynomial character uniquely determine $\gamma(t,\theta)$.

- From transport equation it is easy to establish two identities:

$$\gamma(s,0) \star \gamma(t,0) = \gamma(s+t,0),$$
$$\gamma(t,0) \star \gamma(0,\theta) = \gamma(t,\theta).$$

• Since $\gamma(0,0) = \mathbb{1}$, the first identity shows that, as t varies, $\bar{\alpha}(t) := \gamma(t,0)$ defines a one-parameter subgroup of $\mathcal{G}$. Hence $\bar{\alpha}(t)$ must solve an autonomous equation $(d/dt)\bar{\alpha} = \bar{\alpha} \star \bar{\beta}$, with $\bar{\beta} = (d/dt)\bar{\alpha}(t) \mid_{t=0}$. Furthermore $\bar{\alpha}(t)$ is not oscillatory and intepolates $\alpha(t) = \gamma(t, \omega t)$ at strobocopic times.

• Translate into: $X(t) = W_{\bar{\alpha}(t)}(x_0)$ solves a differential equation $(d/dt)X = W_{\bar{\beta}}(X)$ is not oscillatory and interpolates $x(t)$ at stroboscopic times.

- From the second identity $\bar{\alpha}(t) \star \gamma(0, \omega t) = \alpha(t)$.

- After setting $\kappa(\theta) := \gamma(0, \theta)$, this translates into $x(t) = W_{\kappa(\omega t)}(X(t))$ and we have found the required change of variables.

FINDING THE COEFFICIENTS β AND $\kappa(\theta)$

- Recall these are expressed in terms of $\gamma(t, \theta)$.

- Transport equation used to write recurrence for γ_w, eg for an $n+1$-letter ($n > 0$) word that does not start with the 'letter' 0:

$$\gamma_{k\ell_1\cdots\ell_n} = \frac{i}{k\omega}[\gamma_{\ell_1\cdots\ell_n} - \gamma_{(k+\ell_1)\ell_2\cdots\ell_n}].$$

(Similar formulas obtain for other cases.)

BEYOND FORMAL SERIES. ERROR BOUNDS

• For analytical work, it is necessary to study the convergence of the various series.

• If the series do not converge they have to be truncated. Eg the series for the averaged system $(d/dt)X = W_{\bar{\beta}}(X)$ and change of variables $x = W_{\kappa(\theta)}(X)$ typically do not converge and have to be truncated.

• Under suitable hypothesis the truncations may be carried out to approximate $x(t)$ with errors that are exponentially small in ϵ (Neishtadt (1984), key result in symplectic integration).

• Approach suggested here with simple recursions for the coefficients makes it possible to readily obtain such estimates.

SIMILAR TECHNIQUES

• may be used to analyze some classes of autonomous near integrable systems and to construct (formal) invariant quantities . . .

IIII: EXTENDED WORD SERIES

AN EXAMPLE:

$$\frac{d}{dt}\begin{bmatrix} y \\ \theta \end{bmatrix} = \begin{bmatrix} 0 \\ \omega \end{bmatrix} + f(y,\theta), \quad y \in \mathbb{R}^{D-d}, \omega \in \mathbb{R}^d.$$

θ comprises d angles, f is 2π-periodic in each of the d components of θ, with Fourier coefficients $\widehat{f}_k(y)$, $k \in \mathbb{Z}^d$.

• If f is seen as a perturbation, this is a near integrable system.

• Many system may be written in this form, perhaps after a suitable change of variables.

- Introduce the functions:

$$f_k(y,\theta) = \exp(ik\cdot\theta)\,\hat{f}_k(y), \qquad y\in\mathbb{R}^{D-d},\ \theta\in\mathbb{R}^d,$$

and construct associated word basis functions.

- Solutions are

$$\begin{bmatrix} y_0 \\ \theta_0 \end{bmatrix} + \begin{bmatrix} 0 \\ t\omega \end{bmatrix} + \sum_{n=1}^{\infty} \sum_{k_1,\ldots,k_n} \alpha_{k_1\cdots k_n}(t)\, f_{k_1\cdots k_n}(y_0,\theta_0)$$

(the α's are as before).

DEFINITION:

- If $(v, \delta) \in \mathcal{C} := \mathbb{C}^d \times \mathbb{C}^{\mathcal{W}}$, then its corresponding extended word series is the formal series

$$\overline{W}_{(v,\delta)}(x) = \begin{bmatrix} 0 \\ v \end{bmatrix} + \sum_{w \in \mathcal{W}} \delta_w f_w(x).$$

- Solutions of our system are given by extended word series $\overline{W}_{(t\omega,\alpha(t))}(y_0, \theta_0)$.

THE OPERATION $\bigstar$

- Define for $w = k_1 \cdots k_n \in \mathcal{W}$ the linear operator in $\mathbb{C}^{\mathcal{W}}$

$$(\Xi_v \delta)_w = \exp(i(k_1 + \cdots + k_n) \cdot v)\ \delta_w.$$

- Define the binary operation $\bigstar$ in $\mathcal{C}$

$$(u, \gamma) \bigstar (v, \delta) = (\gamma_\emptyset v + \delta_\emptyset u, \gamma \star (\Xi_u \delta)) \in \mathcal{C}.$$

THE GROUP $\overline{\mathcal{G}}$

- $\overline{\mathcal{G}} = \mathbb{C}^d \times \mathcal{G} \subset \mathcal{C} = \mathbb{C}^d \times \mathbb{C}^{\mathcal{W}}$ is a group for the operation $\bigstar$.

- Acts by composition on extended word series

$$\overline{W}_{(v,\delta)}\big(\overline{W}_{(u,\gamma)}(x)\big) = \overline{W}_{(u,\gamma)\bigstar(v,\delta)}(x), \qquad \gamma \in \mathcal{G}.$$

APPLICATION: SPLITTING

- Given the system:

$$\frac{d}{dt}\begin{bmatrix} y \\ \theta \end{bmatrix} = \begin{bmatrix} 0 \\ \omega \end{bmatrix} + f(y,\theta), \quad y \in \mathbb{R}^{D-d}, \omega \in \mathbb{R}^d,$$

split

$$\frac{d}{dt}\begin{bmatrix} y \\ \theta \end{bmatrix} = \begin{bmatrix} 0 \\ \omega \end{bmatrix}, \qquad \frac{d}{dt}\begin{bmatrix} y \\ \theta \end{bmatrix} = f(y,\theta).$$

• Solutions of split systems corresponds to elements in $\overline{\mathcal{G}}$, hence splitting methods also correspond to elements in this group.

• Order conditions.

• Modified equations valid for ‘large’ time steps.

OTHER APPLICATIONS:

- Normal forms.

- Invariants.