WENDY FOR NONLINEAR ODE

JACK KREBSBACH

1. Strong Form

Given observed data, we wish to estimate the parameters of a D-dimensional system of ordinary differential equations (ODE). This system is assumed to have the form

$$\dot{\boldsymbol{u}} = \boldsymbol{f}(\boldsymbol{p}, \boldsymbol{u}(t), t) \tag{1}$$

where

$$\boldsymbol{u}(t) \in \mathcal{H}^1((0,T), \mathbb{R}^D), \ \boldsymbol{f}(\boldsymbol{p}, \boldsymbol{u}(t), t) = \begin{pmatrix} f_1(\boldsymbol{p}, \boldsymbol{u}(t), t) \\ f_2(\boldsymbol{p}, \boldsymbol{u}(t), t) \\ \vdots \\ f_D(\boldsymbol{p}, \boldsymbol{u}(t), t) \end{pmatrix} \in \mathbb{R}^D \ ^1$$

Note that $\boldsymbol{u}(t)$ is a function of the state variable at time $t \in [0, T]$. The system maybe be Nonlinear in Parameters (NiP).

There are a finite number of parameters $\boldsymbol{p} \in \mathbb{R}^J$ which parameterize $\boldsymbol{f}$. Bold lowercase letters represent vectors while bold uppercase letters represent matrices.

[1] $\mathcal{H}$ is a Sobelev Space

2. Weak Form

To convert from the strong form, Equation 1, to the weak from, we first multiply the right and left sides of the equality element wise with a test function $\boldsymbol{\varphi}_k(t) = \mathbf{1}_D \varphi_k(t)$ where $\varphi_k(t) \in \mathcal{C}_C^\infty((0,T),\mathbb{R})$ and then integrate over the domain $\dot{\boldsymbol{u}}$ and $\boldsymbol{f}$, i.e,

$$\int_0^T \boldsymbol{\varphi}_k(t) \odot \dot{\boldsymbol{u}} \, \mathrm{d}t = \int_0^T \boldsymbol{\varphi}_k(t) \odot \boldsymbol{f} \, \mathrm{d}t^2 \tag{2}$$

Using integration by parts of the lefthand side (LHS) the strong form, Equation 1, becomes

$$\underbrace{\cancel{\boldsymbol{\varphi}(t) \odot \boldsymbol{u}(t)}}_{\mathbf{0}} \Big|_0^T - \int_0^T \dot{\boldsymbol{\varphi}}_k(t) \odot \boldsymbol{u}(t) \, \mathrm{d}t = \int_0^T \boldsymbol{\varphi}_k(t) \odot \boldsymbol{f} \, \mathrm{d}t \tag{3}$$

where the derivative is transfered to the test function. Now the data (state) match the form of the equality. Thus, for a given test function $\boldsymbol{\varphi}(k)(t)$, the weak form of Equation 1 is:

$$-\int_0^T \begin{pmatrix} \dot{\varphi}_k(t) u_1(t) \\ \dot{\varphi}_k(t) u_2(t) \\ \vdots \\ \dot{\varphi}_k(t) u_D(t) \end{pmatrix} \mathrm{d}t = \int_0^T \begin{pmatrix} \varphi_k(t) f_1(\boldsymbol{p}, \boldsymbol{u}(t), t) \\ \varphi_k(t) f_2(\boldsymbol{p}, \boldsymbol{u}(t), t) \\ \vdots \\ \varphi_k(t) f_D(\boldsymbol{p}, \boldsymbol{u}(t), t) \end{pmatrix} \mathrm{d}t$$

Where equality holds for each dimension of the system. Formally, in order for $\boldsymbol{u}(t)$ to be a solution to the weak form of the ODE, it must hold for all possible test functions. In practice, we consider a finite number of test functions. See Section 4 for further interpretation.

[2] $\odot$ is the Hadamard product (element wise multiplication of two vectors)

3. Discretization

We assume that there are M observed state data composed of the true and noise.They are equispaced along the domain $(0, T)$ and take the form

$$\boldsymbol{u}_m = \boldsymbol{u}(t_m) + \boldsymbol{\varepsilon}_m \ \forall m \in \{0, ..., M\}$$

where $\boldsymbol{\varepsilon}_m \overset{\text{i.i.d}}{\sim} \boldsymbol{\mathcal{N}}(\mathbf{0}, \boldsymbol{\Sigma})$.

To satisfy Equation 3 for the set of K test functions we build the following matrices:

$$\boldsymbol{\Phi} = \begin{pmatrix} \varphi_1(t_0) & \varphi_1(t_1) & ... & \varphi_1(t_M) \\ \varphi_2(t_0) & \varphi_1(t_1) & ... & \varphi_2(t_M) \\ \vdots & & \ddots & \\ \varphi_K(t_0) & \varphi_K(t_1) & ... & \varphi_K(t_M) \end{pmatrix} \in \mathbb{R}^{K\times(M+1)}, \dot{\boldsymbol{\Phi}} = \begin{pmatrix} \dot\varphi_1(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_1(t_M) \\ \dot\varphi_2(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_2(t_M) \\ \vdots & & \ddots & \\ \dot\varphi_K(t_0) & \dot\varphi_K(t_1) & ... & \dot\varphi_K(t_M) \end{pmatrix} \in \mathbb{R}^{K\times(M+1)}$$

and the data and right hand side (RHS) we define

$$\boldsymbol{t} := \begin{pmatrix} t_0 \\ t_1 \\ \vdots \\ t_M \end{pmatrix} \in \mathbb{R}^{(M+1)\times 1}, \ \boldsymbol{U} := \begin{pmatrix} \boldsymbol{u}_0^T \\ \vdots \\ \boldsymbol{u}_M^T \end{pmatrix} \in \mathbb{R}^{(M+1)\times D}$$

and

$$\boldsymbol{F} := \begin{pmatrix} \boldsymbol{f}(\boldsymbol{p}, \boldsymbol{u}_0, t_0)^T \\ \vdots \\ \boldsymbol{f}(\boldsymbol{p}, \boldsymbol{u}_M, t_M)^T \end{pmatrix} \in \mathbb{R}^{(M+1)\times D}.$$

To approximate the integrals in Equation 3 for each test function $\varphi_k(t)$ we use Trapezoidal rule, which is equivalent to the following matrix product:

$$-\dot{\boldsymbol{\Phi}}\boldsymbol{U} \approx \boldsymbol{\Phi}\boldsymbol{F}. \tag{4}$$

Because of the compact support means at t_0 and t_M the test functions are zero, so that no quadrature weights are needed (the integral is approximated by summing discrete products).

$$-\dot{\boldsymbol{\Phi}}\boldsymbol{U} = -\begin{pmatrix} \dot\varphi_1(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_1(t_M) \\ \dot\varphi_2(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_2(t_M) \\ \vdots & & \ddots & \\ \dot\varphi_K(t_0) & \dot\varphi_K(t_1) & ... & \dot\varphi_K(t_M) \end{pmatrix} \begin{pmatrix} u_{01} & u_{02} & ... & u_{0D} \\ u_{11} & u_{12} & ... & u_{1D} \\ \vdots & & \ddots & \\ u_{M1} & u_{2M} & ... & u_{MD} \end{pmatrix}$$

$$\boldsymbol{\Phi}\boldsymbol{F} = \begin{pmatrix} \varphi_1(t_0) & \varphi_1(t_1) & ... & \varphi_1(t_M) \\ \varphi_2(t_0) & \varphi_1(t_1) & ... & \varphi_2(t_M) \\ \vdots & & \ddots & \\ \varphi_K(t_0) & \varphi_K(t_1) & ... & \varphi_K(t_M) \end{pmatrix} \begin{pmatrix} f_1(\boldsymbol{p}, \boldsymbol{u}_0, t_0) & ... & f_D(\boldsymbol{p}, \boldsymbol{u}_0, t_0) \\ f_1(\boldsymbol{p}, \boldsymbol{u}_1, t_1) & ... & f_D(\boldsymbol{p}, \boldsymbol{u}_1, t_1) \\ \vdots & \ddots & \\ f_1(\boldsymbol{p}, \boldsymbol{u}_M, t_M) & ... & f_D(\boldsymbol{p}, \boldsymbol{u}_M, t_M) \end{pmatrix}$$

For a given test function $\varphi_k(t)$, the approximation for one dimension of Equation 3 for the LHS and RHS are

$$\begin{aligned} \text{LHS:} \qquad & -\int_0^T \dot\varphi_k(t) u_D(t)\,\mathrm{d}t & &\approx -\sum_{i=0}^{M} \varphi_k(t_i) u_{iD} \\ \text{RHS:} \qquad & \int_0^T \varphi_k(t) f_D(\boldsymbol{p}, \boldsymbol{u}(t), t)\,\mathrm{d}t & &\approx \sum_{i=0}^{M} \varphi_k(t_i) f_D(\boldsymbol{p}, \boldsymbol{u}_i, t_i) \end{aligned}$$

4. Interpretation of Weak Formulation

Inspecting the form of test functions:

$$\varphi_k(t) = C\exp\left(-\frac{9}{\left[1-\left(\frac{t-t_k}{m_t\Delta t}\right)^2\right]_+}\right)$$

we see that instead of using a subscript $\varphi_k(t)$ we can define $\varphi(t) = C\exp\left(-\frac{9}{\left[1-\left(\frac{t}{m_t\Delta t}\right)^2\right]_+}\right)$ and with symmetry

$$\varphi_k(t) = \varphi(t-t_k) \overset{\text{symmetry}}{=} \varphi(t_k - t)$$

Equation 2 becomes

$$(\boldsymbol{\varphi} * \dot{\boldsymbol{u}})(t_k) = \int_0^T \boldsymbol{\varphi}(t_k - t) \odot \dot{\boldsymbol{u}}(t)\,\mathrm{d}t = \int_0^T \boldsymbol{\varphi}(t_k - t) \odot \boldsymbol{f}(\boldsymbol{p}, \boldsymbol{u}(t), t)\,\mathrm{d}t = (\boldsymbol{\varphi} * \boldsymbol{f})(t_k)$$

where $\varphi_k(t)$ is centered about t_k with compact support $\varphi_k \in \mathcal{C}_C^\infty((0,T),\mathbb{R})$, C is chosen such that $\|\varphi_k\|_2 = 1$, and $[\cdot]_+ := \max(\cdot, 0)$. Hence Equation 2 is equivalent to convolving the system with a test function $\boldsymbol{\varphi}_k(t)$ and evaluating at t_k.

What are the forms of allowed for test functions? We want them to be smooth, but what about symmetric? Otherwise does the convolution analogy still work?