WENDY FOR NONLINEAR ODE

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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 $\boldsymbol{u}(t) \in \mathcal{H}^1\big((0,T), \mathbb{R}^D\big)$ ($\mathcal{H}$ is a Sobelev space) 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.

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 with a test function $\varphi_k(t)$, and then integrating over the domain for each dimension of the vector valued functions $\dot{\boldsymbol{u}}$ and $\boldsymbol{f}$, i.e,

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

Notice that that this system is in terms of the derivatives $\dot{\boldsymbol{u}}$, which are unkown. By using integration by parts of the lefthand side (LHS) the strong form, Equation 1, becomes

$$-\int_0^T \dot{\varphi}_k(t)\boldsymbol{u}\,\mathrm{d}t = \int_0^T \varphi_k(t)\boldsymbol{f}\,\mathrm{d}t \tag{3}$$

where the derivative is transfered to the test function. Note that this formulation requires equality for each dimension of the system. That is the product $\dot{\varphi}_k(t)\boldsymbol{u}$ is

$$\dot{\varphi}_k(t)\boldsymbol{u} = [\dot{\varphi}_k(t)u_1(t),\ \dot{\varphi}_k(t)u_2(t),\ \dots\ ,\ \dot{\varphi}_k(t)u_D(t)]^T \in \mathbb{R}^D$$

and

$$\varphi_k(t)\boldsymbol{f} = [\varphi_k(t)f_1(\boldsymbol{p},\boldsymbol{u}(t),t),\ \varphi_k(t)f_2(\boldsymbol{p},\boldsymbol{u}(t),t),\ \dots\ ,\ \varphi_k(t)f_D(\boldsymbol{p},\boldsymbol{u}(t),t)]^T \in \mathbb{R}^D.$$

Thus, for a given test function $\varphi_k(t)$, 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.

3. Discretization

We assume that there are M observed state data, which are equispaced along the domain $(0, T)$ and is of the form

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

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).

$$-\dot{\boldsymbol{\Phi}}\boldsymbol{U} = -\begin{pmatrix} \dot\varphi_1(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_1(t_M) \\ \dot\varphi_2(t_0) & \dot\varphi_1(t_1) & ... & \dot\varphi_2(t_M) \\ \vdots & & \ddots & \\ \dot\varphi_K(t_0) & \dot\varphi_K(t_1) & ... & \dot\varphi_K(t_M) \end{pmatrix} \begin{pmatrix} u_1(t_0) & u_2(t_0) & ... & u_D(t_0) \\ u_1(t_1) & u_2(t_1) & ... & u_D(t_1) \\ \vdots & & \ddots & \\ u_1(t_M) & u_2(t_M) & ... & u_D(t_M) \end{pmatrix}$$

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

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

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

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 taking advantage of symmetry

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

and Equation 2 becomes

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

Note that $\varphi_k(t)$ 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 $[\cdot]_+ := \max(\cdot, 0)$. So the Equation 2 is equivalent to convolving the system with a test function $\varphi(t)$.

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?