MTH 410/510 II: Final Project, due by noon on 03/21/2019

Estimation of distributed source parameters for a nonlinear dynamical system

The goal of this project is to apply constrained optimization techniques for estimating space-distributed source parameters (forcing term) in a nonlinear dynamical system. Issues related with parameter estimation (identifiability) are also illustrated.

SETUP. Consider the initial-boundary value problem (IBVP) for the function $u(x,t)$,

$$\begin{cases} u_t(x,t) - u_{xx}(x,t) + u^3(x,t) = \alpha(x), & \forall 0 < x < 1, \ \forall t > 0 \\ u(0,t) = 0, \quad u(1,t) = 0, & \forall t > 0 \\ u(x,0) = u_0(x), & 0 \le x \le 1 \end{cases} \tag{1}$$

Physically, the IBVP problem (1) models a diffusion process $u_t - u_{xx}$ with a nonlinear reaction term u^3, and a space-dependent parameter (source/forcing term), $\alpha(x)$. The initial state $u_0(x)$ at time $t_0 = 0$ is assumed to be known. In this assignment we want to find an optimal **space-distributed** parameter $\alpha^\star$ such that the solution to (1) is as close as possible to a given function (desired outcome/goal, measurement) $\bar{u}(x)$, as explained below.

A discrete version to the IBVP (1) is obtained by considering a uniform partition of the spatial domain [0, 1] with nodes $\{x_i : i = 0 : n+1\}$ at an increment $h = 1/(n+1)$,

$$0 = x_0 < x_1 < \ldots < x_n < x_{n+1} = 1, \quad x_i = i * h, \ \text{for } i = 0 : n+1$$

and a time increment (step) $\Delta t = k$ to advance the state in time from $t_0 = 0$,

$$t_j = t_{j-1} + k, \quad \text{for } j = 1, 2, \ldots$$

The second-order derivative in space is approximated as

$$u_{xx}(x_i, t_j) \approx \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2}, \quad i = 1 : n, \ j \ge 0 \tag{2}$$

and the first-order time derivative is approximated as

$$u_t(x_i, t_j) \approx \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k}, \quad i = 1 : n, \ j \ge 0 \tag{3}$$

The discrete version to the IBVP (1) for $u_{i,j} \approx u(x_i, t_j), i = 1 : n, \ j = 0, 1, \ldots$ is obtained as

$$\begin{cases} \dfrac{u_{i,j+1} - u_{i,j}}{k} - \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + u_{i,j}^3 = \alpha_i, \quad i = 1 : n, \ j = 0, 1, \ldots \\ u_{0,j} = 0, \quad u_{n+1,j} = 0, \ j = 1, 2, \ldots \ \text{(boundary condition)} \\ u_{i,0} = u_0(x_i), \ i = 0 : n+1, \ \text{(initial condition)} \end{cases} \tag{4}$$

where $\alpha_i = \alpha(x_i), i = 1 : n$.

THE DISCRETE DYNAMICAL SYSTEM. In a compact format, the system of equations (4) to advance the state from time t_{j-1} to time t_j is written

$$\mathbf{u}_j = \mathbf{A}\mathbf{u}_{j-1} - k\mathbf{F}(\mathbf{u}_{j-1}) + k\boldsymbol{\alpha}, \quad j = 1, 2, \ldots \tag{5}$$

where the notation is as follows:

$$\mathbf{A} \in \mathbb{R}^{n\times n},\ \mathbf{A} = \begin{pmatrix} 1-2s & s & & 0 \\ s & \ddots & \ddots & \\ & \ddots & \ddots & s \\ 0 & & s & 1-2s \end{pmatrix},\quad s \overset{def}{=} \frac{k}{h^2}$$

$$\mathbf{u}_j \in \mathbb{R}^n,\ \mathbf{u}_j = \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{n,j} \end{bmatrix}, j = 0, 1, \ldots;\ \boldsymbol{\alpha} \in \mathbb{R}^n,\ \boldsymbol{\alpha} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{bmatrix},\ \mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n,\ \mathbf{F}(\mathbf{u}) = \begin{bmatrix} u_1^3 \\ u_2^3 \\ \vdots \\ u_n^3 \end{bmatrix}$$

THE OPTIMIZATION PROBLEM. With a specified initial condition $\mathbf{u}_0$, the discrete system (5) defines the time evolution of the state vector $\mathbf{u}$ as a function of the parameter vector $\boldsymbol{\alpha}$. Optimal parameter values $\boldsymbol{\alpha}^\star \in \mathbb{R}^n$ are obtained by minimizing the distance between the model predicted state $\mathbf{u}_m$ at time t_m and a data set $\widetilde{\mathbf{u}}_m$ (measurements or goal values) specified at time t_m. The optimality criteria is formulated as a constrained optimization problem,

$$\min_{[\boldsymbol{\alpha},\mathbf{u}_1,\mathbf{u}_2,\ldots\mathbf{u}_m]} \frac{1}{2}\|\mathbf{u}_m - \widetilde{\mathbf{u}}_m\|^2 \tag{6}$$

subject to the constraints

$$\mathbf{u}_j = \mathbf{A}\mathbf{u}_{j-1} - k\mathbf{F}(\mathbf{u}_{j-1}) + k\boldsymbol{\alpha}, \quad j = 1 : m \tag{7}$$

Notice that in this formulation the number of parameters is $(n + m \times n)$. The Lagrangian function is $\mathscr{L} : \mathbb{R}^n \times \mathbb{R}^{n\times m} \times \mathbb{R}^{n\times m}$,

$$\mathscr{L}(\boldsymbol{\alpha}, \mathbf{u}, \boldsymbol{\lambda}) = \frac{1}{2}\|\mathbf{u}_m - \widetilde{\mathbf{u}}_m\|^2 - \sum_{j=1}^{m} \boldsymbol{\lambda}_j^{\mathrm{T}} \cdot [\mathbf{u}_j - \mathbf{A}\mathbf{u}_{j-1} + k\mathbf{F}(\mathbf{u}_{j-1}) - k\boldsymbol{\alpha}] \tag{8}$$

where $\mathbf{u} = [\mathbf{u}_1, \mathbf{u}_2, \ldots \mathbf{u}_m]$ is the time-series of the model state, $\boldsymbol{\lambda}_j \in \mathbb{R}^n$ denotes the vector of Lagrange variables at time $t_j, j = 1 : m$ and $\boldsymbol{\lambda} = [\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots \boldsymbol{\lambda}_m] \in \mathbb{R}^{n\times m}$.

First-order optimality conditions are

$$\nabla_{\mathbf{u}_m}\mathscr{L} = \mathbf{u}_m - \widetilde{\mathbf{u}}_m - \boldsymbol{\lambda}_m \quad = \quad \mathbf{0} \tag{9}$$

$$\nabla_{\mathbf{u}_j}\mathscr{L} = -\boldsymbol{\lambda}_j + [\mathbf{A} - k\mathbf{F}'(\mathbf{u}_j)]^{\mathrm{T}} \boldsymbol{\lambda}_{j+1} \quad = \quad \mathbf{0}, \quad j = m-1 : -1 : 1 \tag{10}$$

$$\nabla_{\boldsymbol{\alpha}}\mathscr{L} = k\sum_{j=1}^{m} \boldsymbol{\lambda}_j \quad = \quad \mathbf{0} \tag{11}$$

where $\mathbf{F}'(\mathbf{u})$ denotes the Jacobian matrix of $\mathbf{F}(\mathbf{u})$, here a diagonal matrix, $\mathbf{F}'(\mathbf{u}) = diag(3\mathbf{u}.^2)$.

Alternatively, we may formulate an unconstrained optimization problem, by using the model equations (5) to express $\mathbf{u}_m$ in terms of the input parameters $\boldsymbol{\alpha}$. The reduced problem is

$$\boldsymbol{\alpha}^\star = \arg\min_{\boldsymbol{\alpha}} f(\boldsymbol{\alpha}), \quad f(\boldsymbol{\alpha}) \stackrel{def}{=} \frac{1}{2}\|\mathbf{u}_m(\boldsymbol{\alpha}) - \widetilde{\mathbf{u}}_m\|^2 \tag{12}$$

The gradient of the cost functional (12), $\nabla_{\boldsymbol{\alpha}} f(\boldsymbol{\alpha})$, may be evaluated as follows:

Backward Integration (Adjoint Model):

$$\boldsymbol{\lambda}_m \stackrel{def}{=} \mathbf{u}_m - \widetilde{\mathbf{u}}_m \tag{13}$$

$$\text{for } j = m-1 : -1 : 1 \tag{14}$$

$$\quad \boldsymbol{\lambda}_j \stackrel{def}{=} \left[\mathbf{A} - k\mathbf{F}'(\mathbf{u}_j)\right]^{\mathrm{T}} \boldsymbol{\lambda}_{j+1} \tag{15}$$

$$\text{end} \tag{16}$$

$$\nabla_{\boldsymbol{\alpha}} f(\boldsymbol{\alpha}) = k\sum_{j=1}^{m} \boldsymbol{\lambda}_j \tag{17}$$

PROJECT DATA. The data to implement this project is specified as follows.

- initial condition: $u_0(x) = \sin(2\pi x)$.
- dimension of the state vector: $n = 49$; this gives an x-increment of $h = 1/(n+1) = 0.02$
- time step: $k = 0.5h^2$ (thus $s = 0.5$) and number of time steps: $m = 100$
- $\widetilde{\mathbf{u}}_m$ data at time t_m: given in data file *prdata*1.*m*
- $\widetilde{\mathbf{u}}_{2m}$ validation data at time t_{2m} (see below why needed): given in data file *prdata*2.*m*

PROJECT TASKS

Task 1 (10 points). Implement a function $\mathbf{u} = ibvpmodel(n, m, h, \boldsymbol{\alpha}, \mathbf{u}_0)$ that takes as input a parameter vector $\boldsymbol{\alpha}$, an initial condition $\mathbf{u}_0$, the state dimension n, the number of time steps m, and the grid parameter h and returns the time-distributed state $\mathbf{u}$ obtained from equations (7) with $k = 0.5h^2$.

Task 2 (80 points). Use a method of your choice to find the optimal parameters $\boldsymbol{\alpha}^\star \in \mathbb{R}^n$ and the associated time-series of states $\mathbf{u}^\star$ by solving (6-7) or the reduced problem (12). Provide:

- The plot (spatial distribution) of the optimal parameter values $\boldsymbol{\alpha}^\star$.
- The plot of the model state $\mathbf{u}_m^\star$ fit to data $\widetilde{\mathbf{u}}_m$ at time t_m.
- The value of cost function $f(\boldsymbol{\alpha}^\star)$.
- *Validation procedure*: The plot of the model state $\mathbf{u}_{2m}^\star$ fit to data $\widetilde{\mathbf{u}}_{2m}$ at time t_{2m}.

Task 3 (10 points). Repeat the experiments at **Task 2** but using the initial condition $u_0(x) = \sin(\pi x)$. Comment on your results.

Attach a listing/hardcopy of the codes used to implement the functions at Tasks 1 and 2.