MTH 465/565: Homework #4 - due on March 8, 2023

Parameter estimation for a nonlinear boundary value problem

Setup. Consider the nonlinear boundary value problem (BVP) for a function $u : [0,\ 1] \to \mathbb{R}$,

$$\begin{cases} -u''(x) + u^3(x) = \alpha \\ u(0) = 0, \quad u(1) = 0 \end{cases} \tag{1}$$

where $\alpha \in \mathbb{R}$ is a constant scalar parameter. In this assignment we want to find an optimal value $\alpha^\star$ of the parameter α such that the solution $u(x)$ 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 BVP (1) is obtained by considering a uniform partition of the interval $[0,\ 1]$ 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 an approximation of the second order derivative using a finite difference formula with error $O(h^2)$,

$$u''(x_i) \approx \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}, \quad i = 1 : n \tag{2}$$

The discrete version to the BVP (1) is obtained as

$$\begin{cases} -\dfrac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + u_i^3 = \alpha, \quad i = 1 : n \\ u_0 = 0, \quad u_{n+1} = 0 \end{cases} \tag{3}$$

where $u_i \approx u(x_i), i = 1 : n$. In a compact format, the system of equations (3) is written

$$\mathbf{A}\mathbf{u} + \mathbf{G}(\mathbf{u}) = \alpha \mathbf{1}_n \tag{4}$$

where the notation is as follows:

$$\mathbf{u} \in \mathbb{R}^n,\ \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}, \quad \mathbf{A} \in \mathbb{R}^{n\times n},\ \mathbf{A} = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & 0 \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 2 \end{pmatrix}$$

$$\mathbf{1}_n \in \mathbb{R}^n,\ \mathbf{1}_n = \begin{bmatrix} 1 \\ \vdots \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{G} : \mathbb{R}^n \to \mathbb{R}^n,\ \mathbf{G}(\mathbf{u}) = \begin{bmatrix} u_1^3 \\ u_2^3 \\ \vdots \\ u_n^3 \end{bmatrix}$$

We look for the optimal parameter $\alpha^\star$ and the associated solution $\mathbf{u}^\star$ to the discrete BVP using Lagrange multipliers theory. Consider the constrained optimization problem

$$\min_{(\mathbf{u},\alpha)} f(\mathbf{u}, \alpha), \quad f(\mathbf{u}, \alpha) \stackrel{def}{=} \frac{1}{2}\|\mathbf{u} - \bar{\mathbf{u}}\|^2 \tag{5}$$

subject to the constraints given by the n-equations of the discrete BVP

$$\mathbf{A}\mathbf{u} + \mathbf{G}(\mathbf{u}) - \alpha \mathbf{1}_n = \mathbf{0} \tag{6}$$

The Lagrangian function is $\mathscr{L} : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^n \longrightarrow \mathbb{R}$,

$$\mathscr{L}(\mathbf{u}, \alpha, \boldsymbol{\lambda}) = \frac{1}{2}\|\mathbf{u} - \bar{\mathbf{u}}\|^2 - \boldsymbol{\lambda}^{\mathrm{T}} \cdot [\mathbf{A}\mathbf{u} + \mathbf{G}(\mathbf{u}) - \alpha \mathbf{1}_n] \tag{7}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^n$ is the vector of Lagrange multipliers. The system of first-order optimality equations for the constrained optimization problem (5), (6) has $(2n+1)$ equations:

$$\left\{ \begin{array}{lclll} \nabla_{\mathbf{u}} \mathscr{L}(\alpha^\star, \mathbf{u}^\star, \boldsymbol{\lambda}^\star) & = & \mathbf{0} & \rightarrow n\, equations: & \mathbf{u} - \bar{\mathbf{u}} - (\mathbf{A} + \mathbf{G}'(\mathbf{u}))^{\mathrm{T}} \boldsymbol{\lambda} = \mathbf{0} \\ \nabla_{\alpha} \mathscr{L}(\alpha^\star, \mathbf{u}^\star, \boldsymbol{\lambda}^\star) & = & 0 & \rightarrow 1\, equation: & \mathbf{1}_n^{\mathrm{T}} \boldsymbol{\lambda} = 0 \\ \nabla_{\boldsymbol{\lambda}} \mathscr{L}(\alpha^\star, \mathbf{u}^\star, \boldsymbol{\lambda}^\star) & = & \mathbf{0} & \rightarrow n\, equations & \mathbf{A}\mathbf{u} + \mathbf{G}(\mathbf{u}) - \alpha \mathbf{1}_n = \mathbf{0} \end{array} \right. \tag{8}$$

where $\mathbf{G}'(\mathbf{u})$ denotes the Jacobian matrix of $\mathbf{G}(\mathbf{u})$, here a diagonal matrix with diagonal entries $3u_i^2, i = 1:n$.

<u>Your job</u>

Task 1 (20 points). Write a function

$$[\alpha^\star, \mathbf{u}^\star, \boldsymbol{\lambda}^\star, f^\star] = lmbvpoptim(n, \bar{\mathbf{u}})$$

that takes as input the number of interior nodes n and the n-dimensional data vector $\bar{\mathbf{u}}$ and returns the optimal parameter value $\alpha^\star$, the optimal $n-$dimensional state vector $\mathbf{u}^\star$, the vector of Lagrange multipliers $\boldsymbol{\lambda}^\star$, and the corresponding value of the cost functional defined in (5), $f^\star \stackrel{def}{=} f(\mathbf{u}^\star, \alpha^\star)$. Your function *lmbvpoptim* may use a build-in function such as *fsolve* to provide the solution to the first order optimality system.

Task 2 (20 points). Test your code using $n = 99$ and for each of the data functions

$$(a)\ \bar{u}(x) = \sin(\pi x)\,; \qquad (b)\ \bar{u}(x) = \sin^2(2\pi x)$$

Things to hand in:

- Listing/hardcopy of the cods used to implement the function at Task 1.
- For each test run, provide the numerical outcomes from Task 2: the corresponding values of $\alpha^\star, f(\mathbf{u}^\star, \alpha^\star)$ and show the graph of $\mathbf{u}^\star$ as compared with the data $\bar{\mathbf{u}}$.
  In addition, for each test run, provide a graph/plot of the vector of Lagrange multipliers $\boldsymbol{\lambda}^\star$. What is the interpretation of the plot of $\boldsymbol{\lambda}^\star$?