Parameter identification with ODE models

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1 Parameter estimation problem

We consider a smooth n-dimsniosnal ODE depending on parameters $p \in \mathbb{R}^{n_p}$

$$u_t(t) = f(p, u(t)) + l(p, t), \quad t \in I =]0, T[, \qquad u(0) = u_0(p) \tag{1}$$

with weak formulation

$$u \in H^1(I, \mathbb{R}^n): \quad a(p, u)(v, v_0) = b(p)(v, v_0) \quad \forall (v, v_0) \in L^2(I, \mathbb{R}^n) \times \mathbb{R}^n \tag{2}$$

with

$$a(p, u)(v, v_0) := \int_0^T \langle u_t - f(p, u), v\rangle + \langle u(0), v_0\rangle, \quad b(p)(v, v_0) = \int_0^T \langle l(p), v\rangle + \langle u_0(p), v_0\rangle. \tag{3}$$

We consider the least-squares problem

$$J(p,u) = \frac{1}{2}\|R(u)\|^2 + \frac{\alpha}{2}\|p-p_0\|^2, \quad R(u) := C(u) - C_0 \tag{4}$$

where $C : H^1(I,\mathbb{R}^n) \to \mathbb{R}^{n_C}$ is a bounded linear observation operator. We suppose that (1) admits a unique solution $u(p)$ and introduce the reduced functional

$$\hat{J}(p) := J(p,u(p)), \quad \hat{C}(p) := C(u(p)). \tag{5}$$

We have

$$\langle \nabla\hat{J}(p), q\rangle = \langle \hat{R}(p), \hat{C}'(p)(q)\rangle + \alpha\langle p-p_0, q\rangle \tag{6}$$

where $\delta u \in H^1(I,\mathbb{R}^n)$ solves for all $(v,v_0) \in L^2(I,\mathbb{R}^n)\times\mathbb{R}^n$

$$a'_u(p,u)(\delta u, v, v_0) = b'_p(p)(q,v,v_0) - a'_p(p,u)(q,v,v_0). \tag{7}$$

2 FEM discretization

We let $\delta = (0 = t_0 < t_1 < \cdots < t_N = T)$ be a partition, $I_k :=]t_{k-1}, t_k[$, $\delta_k =: t_k - t_{k-1}$, $1 \leqslant k \leqslant N$. Let $U_\delta \subset H^1(I,\mathbb{R}^n)$ and $V_\delta \subset L^2(I,\mathbb{R}^n)$ be conforming finite element spaces. We denote by $\tilde{u} \in U_\delta$ a linearization point in order to obtain semi-implicit schemes:

$$a_\delta(p,u)(v) := \int_0^T \langle u' - (f(p,\tilde{u}) + f'_u(p,\tilde{u})(u-\tilde{u})), v\rangle \tag{8}$$

$$\tilde{u}_{|_{I_k}} := u(t_{k-1}) \tag{9}$$

We have

$$a_\delta{}'_u(p,u)(w,v) := \int_0^T \langle w' - (f'_u(p,\tilde{u})(w) + f''_{uu}(p,\tilde{u})(\tilde{w}, u-\tilde{u})), v\rangle \tag{10}$$

3 General parameter estimation problem

We consider the state equation

$$u \in U: \; a(p,u)(v) = l(p)(v) \quad \forall v \in V. \tag{11}$$

We suppose that (11) has a unique solution $u = u(p)$.

We consider the least-squares problem of minimizing with linear continuous $C : U \to Z$

$$J(p) = \frac{1}{2}\|R(p)\|^2 + \frac{\alpha_{LM}}{2}\|p-\overline{p}\|^2, \quad R(p) := C(u(p)) - \overline{C}. \tag{12}$$

Based on conforming discretizations, we let

$$U_\delta \subset U, \quad V_\delta \subset V, \quad \dim U_\delta = \dim V_\delta = N_\delta.$$

we define the discrete problems

$$u_\delta \in U_\delta : \; a(p, u_\delta)(v) = l(p)(v) \quad \forall v \in V_\delta. \tag{13}$$

Then assuming unique solvability, we let $u_\delta = u_\delta(p)$. Then we have the discrete least-squares problem of minimizing

$$J_\delta(p) = \frac{1}{2}\|R_\delta(p)\|^2 + \frac{\alpha_{LM}}{2}\|p - \overline{p}\|^2, \quad R_\delta(p) := C(u_\delta(p)) - \overline{C}. \tag{14}$$

Let $u' = u'(p)(q) \in U$ solve for all $v \in V$

$$a'_u(p, u)(u', v) = l'_p(p)(q, v) - a'_u(p, u)(q, v) \tag{15}$$

and

$$z \in V : \; a'_u(p, u)(w, z) = C(w) \quad \forall w \in U. \tag{16}$$

as well as $u'_\delta \in U_\delta$ and $z_\delta \in V_\delta$ the corresponding Petrov-Galerkin solutions.

Lemma 1.

$$J(p) - J_\delta(p) \leqslant \|C(u(p) - u_\delta(p))\| \left(\frac{1}{2}\|C(u(p) - u_\delta(p))\| + \|R_\delta(p)\|\right) \tag{17}$$

$$\begin{aligned}\|\nabla J(p) - \nabla J_\delta(p)\| \leqslant & \|C(u(p) - u_\delta(p))\| \left(\|C(u'(p))\| + \|C(u'(p) - u'_\delta(p))\|\right) \\ & + \|R_\delta(p)\| \, \|C(u'(p) - u'_\delta(p))\|.\end{aligned} \tag{18}$$

Proof.

$$\begin{aligned} J(p) - J_\delta(p) =& \frac{1}{2}\|R(p)\|^2 - \frac{1}{2}\|R_\delta(p)\|^2 = \frac{1}{2}\|R(p) - R_\delta(p)\|^2 + \langle R(p) - R_\delta(p), R_\delta(p)\rangle \\ =& \frac{1}{2}\|C(u(p) - u_\delta(p))\|^2 + \langle C(u(p) - u_\delta(p)), R_\delta(p)\rangle \end{aligned}$$

and

$$\begin{aligned} \langle \nabla J(p) - \nabla J_\delta(p), q\rangle =& \langle R(p), C(u'(p)(q))\rangle - \langle R_\delta(p), C(u'_\delta(p)(q))\rangle \\ =& \langle C(u(p) - u_\delta(p)), C(u'(p)(q))\rangle + \langle R_\delta(p), C(u'(p)(q) - u'_\delta(p)(q))\rangle \end{aligned}$$

□

[1]

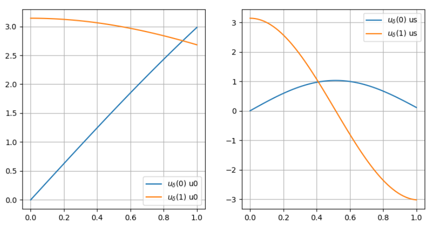
4 Numerical experiments

4.1 Bock's example

[2]

$$\begin{bmatrix} u' \\ v' \end{bmatrix} = \begin{bmatrix} v \\ -pu \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ v(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad C = \begin{bmatrix} u(T) \\ \int_0^T u(t) \end{bmatrix}, \quad \overline{C} = \begin{bmatrix} 0 \\ 2/\pi \end{bmatrix} \tag{19}$$

with $T = 1$. We use an initial guess $p_0 = 1$. The solution is $p^* = \pi$.



```
it       J           G         eta         ref
==========================================
 1 4.84880e+00 1.4772e+00 1.1052e-03
 2 4.59778e-05 1.6792e-02 1.1701e-03
 3 1.46571e-05 4.6083e-06 1.1701e-03  *
 4 1.72445e-06 3.8771e-03 7.3136e-05
 5 1.71652e-06 3.8679e-03 7.3136e-05
 6 1.70079e-06 3.8496e-03 7.3136e-05
 7 1.66986e-06 3.8133e-03 7.3136e-05
 8 1.60999e-06 3.7421e-03 7.3136e-05
 9 1.49784e-06 3.6049e-03 7.3136e-05
10 1.30053e-06 3.3499e-03 7.3136e-05
11 9.49305e-07 2.8399e-03 7.3136e-05
12 4.20493e-07 1.8199e-03 7.3136e-05
13 5.20125e-08 3.4296e-08 7.3136e-05  *
14 5.89610e-09 2.2629e-04 4.5711e-06
15 5.89265e-09 2.2622e-04 4.5711e-06
16 5.88575e-09 2.2609e-04 4.5711e-06
17 5.87198e-09 2.2581e-04 4.5711e-06
18 5.84456e-09 2.2527e-04 4.5711e-06
19 5.79017e-09 2.2418e-04 4.5711e-06
20 5.68324e-09 2.2202e-04 4.5711e-06
21 5.47643e-09 2.1780e-04 4.5711e-06
22 5.08945e-09 2.0966e-04 4.5711e-06
23 4.41029e-09 1.9456e-04 4.5711e-06
24 3.20419e-09 1.6436e-04 4.5711e-06
25 1.40089e-09 1.0396e-04 4.5711e-06
26 1.98365e-10 1.1791e-10 4.5711e-06  *
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x0=1 xs=array([3.14158935])
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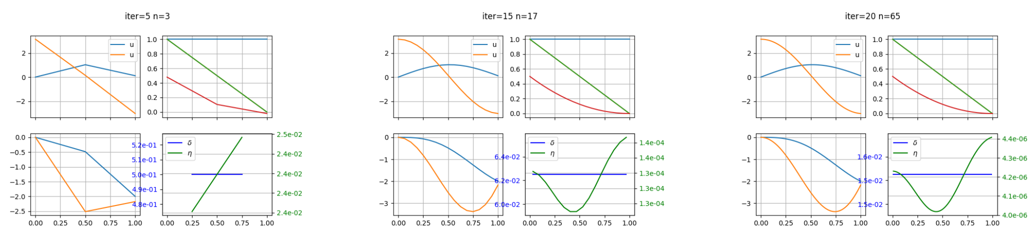
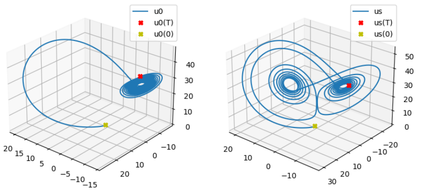


Figure 1: Bock's example



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it         J            G        eta          ref
==========================================
  1 2.22043e+00 1.6058e+01 1.1440e+00
  2 2.22043e+00 1.6058e+01 1.1440e+00
  3 1.10660e+00 8.8892e+00 1.0170e+00  *
  4 6.10426e-01 6.4076e+00 2.9267e-01
  5 2.57022e-01 3.1981e+00 3.2800e-01  *
  6 2.22454e-01 5.1915e-01 8.3001e-02  *
  7 2.22383e-01 3.0083e-01 2.0960e-02
  8 2.22065e-01 4.5195e-03 2.0933e-02  *
info['nfev']=20 info['njev']=7 success=2
x0=array([0.1]) xs=array([0.32222869])
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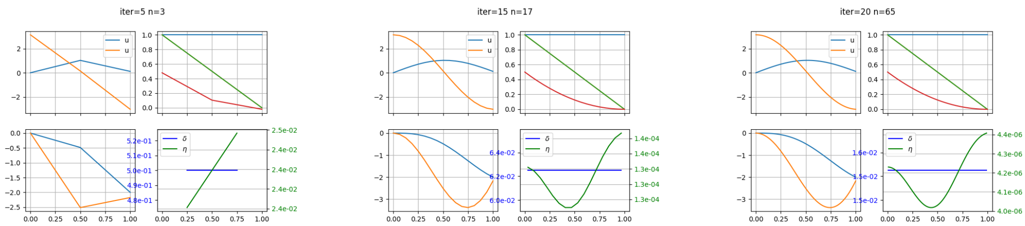


Figure 2: Bock's example

4.2 Lorenz

4.3 Oscillator

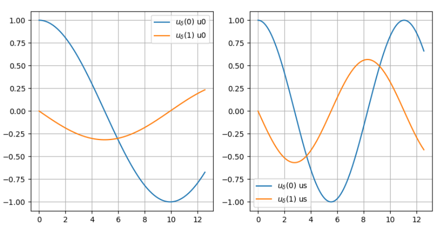
$$\begin{bmatrix} u' \\ v' \end{bmatrix} = \begin{bmatrix} v \\ -pu \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ v(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad C = \begin{bmatrix} u(T) \\ v(T) \end{bmatrix}, \quad \overline{C} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{20}$$

with $T = 12$. We use an initial guess $p_0 = 0.1$. The closest solution is $p^* \approx 0.322$.

References

[1] M. Feischl, "Inf-sup stability implies quasi-orthogonality," *Math. Comp.*, vol. 91, no. 337, pp. 2059–2094, 2022.

[2] H. G. Bock, *Randwertproblemmethoden zur Parameteridentifizierung in Systemen nichtlinearer Differentialgleichungen*, vol. 183 of *Bonner Mathematische Schriften [Bonn Mathematical Publications]*. Universität Bonn, Mathematisches Institut, Bonn, 1987. Dissertation, Rheinische Friedrich-Wilhelms-Universität, Bonn, 1985.



```
it        J            G        eta          ref
========================================
  1 2.22043e+00 1.6058e+01 1.1440e+00
  2 2.22043e+00 1.6058e+01 1.1440e+00
  3 1.10660e+00 8.8892e+00 1.0170e+00  *
  4 6.10426e-01 6.4076e+00 2.9267e-01
  5 2.57022e-01 3.1981e+00 3.2800e-01  *
  6 2.22454e-01 5.1915e-01 8.3001e-02  *
  7 2.22383e-01 3.0083e-01 2.0960e-02
  8 2.22065e-01 4.5195e-03 2.0933e-02  *
info['nfev']=20 info['njev']=7 success=2
x0=array([0.1]) xs=array([0.32222869])
```

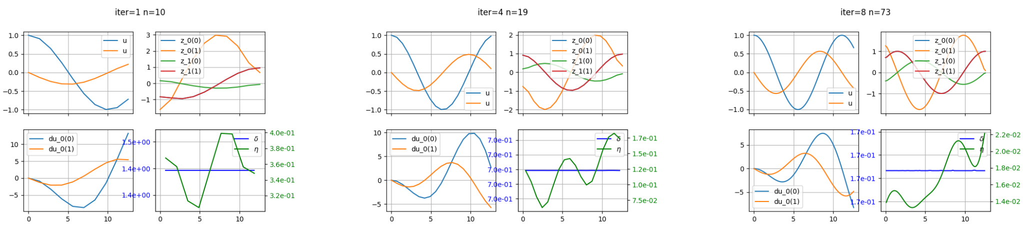


Figure 3: default