Math 540: Project 2

Due Tuesday, February 26

1. We show in Example 3.5 that the boundary value problem

$$\frac{d^2T_s}{dx^2} = \frac{2(a+b)}{ab}\frac{h}{k}\left[T_s(x) - T_{amb}\right]$$
$$\frac{dT_s}{dx}(0) = \frac{\Phi}{k} \quad , \quad \frac{dT_s}{dx}(L) = \frac{h}{k}[T_{amb} - T_s(L)]$$

models the steady state temperature $T_s(x)$ of an uninsulated rod with source heat flux Φ at $x = 0$ and ambient air temperature T_{amb}. The model parameters are $q = [\Phi, h, k]$, where h is the convective heat transfer coefficient and k is the thermal conductivity.

The analytic solution is

$$y(x, q) = T_s(x, q) = c_1(q)e^{-\gamma x} + c_2(q)e^{\gamma x} + T_{amb},$$

where $\gamma = \sqrt{\frac{2(a+b)h}{abk}}$ and

$$c_1(q) = -\frac{\Phi}{k\gamma}\left[\frac{e^{\gamma L}(h + k\gamma)}{e^{-\gamma L}(h - k\gamma) + e^{\gamma L}(h + k\gamma)}\right] \quad , \quad c_2(q) = \frac{\Phi}{k\gamma} + c_1(q).$$

We suppress the parameter dependence of γ to clarify the notation. In Chapter 7, we will estimate the parameter values $k = 2.37, h = 0.00191$ and $\Phi = -18.4$, which you can use here. The measured ambient room temperature is $T_{amb} = 21.29^o$C and the rod has cross-sectional dimensions $a = b = 0.95$ cm and length $L = 70$ cm.

(a) Use finite-differences to approximate the sensitivity relations $\frac{\partial y}{\partial \Phi}$, $\frac{\partial y}{\partial h}$ and $\frac{\partial y}{\partial k}$ and plot your solutions at the 15 equally spaced spatial locations $x_i = x_0 + (i-1)\Delta x$, where $x_0 = 10$ cm and $\Delta x = 4$ cm. Use a discrete line-type so your plot looks like Figure 7.4. Additionally, compute the analytic sensitivity relation $\frac{\partial y}{\partial \Phi}$ and plot with your finite-difference solution to compare their accuracy. If you have time, compute and compare the analytic sensitivities for h and k.

(b) For the parameters $q = [\Phi, h, k]$, construct the sensitivity matrix $\chi_{ij}(q) = \frac{\partial y(x_i,q)}{\partial q_j}$ and the matrix $V = \chi^T\chi$. Compute the rank of V and discuss the identifiability of the complete parameter set. Discuss why you can deduce this result based on the model.

(c) As detailed in the text, the thermal conductivity k is well-documented for aluminum and copper. Fix this parameter and repeat your analysis for the parameters $q = [\Phi, h]$. Are they identifiable?

2. Consider the Helmholtz energy

$$\psi(P, q) = \alpha_1 P^2 + \alpha_{11}P^4 + \alpha_{111}P^6,$$

where P is the polarization and $q = [\alpha_1, \alpha_{11}, \alpha_{111}]$ are parameters. You can take nominal values to be $\alpha_1 = -389.4, \alpha_{11} = 761.3$ and $\alpha_{111} = 61.5$. When sampling for global sensitivity analysis, you should sample each parameter from $\mathcal{U}(0, 1)$ and map to the interval $[\alpha_\ell, \alpha_r]$ that is 20% above and below the nominal value. For uniformly sampling on the interval $[a, b]$, one would use the command `q = a + (b-a)*rand(1,1)`.

(a) Plot the energy for P in the interval $[-0.8, 0.8]$. Do you observe the double-well behavior?

(b) Analytically compute the sensitivity matrix χ and matrix $V = \chi^T \chi$ using 17 equally spaced polarization values in the domain $[0, 0.8]$. Compute the rank of V and discuss the identifiability of the parameters q.

(c) Use Morris screening with forward differences and $r = 50, \Delta = 1/20$, to compute μ_i^* and σ_i^2. You can use the scalar response

$$y(q) = \int_0^{0.8} \psi(P, q) dP, \tag{1}$$

which you can compute analytically. To check your solution, show that $\mu^* \approx \left[\frac{\partial y}{\partial \alpha_1}, \frac{\partial y}{\partial \alpha_{11}}, \frac{\partial y}{\partial \alpha_{111}}\right]$. Explain why you would expect $\sigma_i^2 \approx 0$ for a linearly parameterized problem such as this one. Which parameter is least influential?

(d) Use the Saltelli algorithm 15.10.1 to approximate the Sobol sensitivity indices S_i and S_{T_i}. Show that

$$\sum_{i=1}^{3} S_i \approx 1.$$

What does this indicate about the second-order effects S_{ij} and is this to be expected for a linearly parameterized problem? Use `kde.m` to plot a kernel density estimate of y_A computed in Step 3 of the algorithm. Now fix any noninfluential parameters at their nominal values and recompute y_A. Plot the new kde on the same plot as the 3-parameter case and discuss your results and determine if there is a discrepancy with (b). We will revisit this problem when we do Bayesian inference.

3. Exercise 15.5: *Do only the Saltelli-Sobol analysis.* You can use the following commands to numerically solve the ode and approximate the integral. Here `A` is the matrix in the Saltelli algorithm.

```
tf = 5;
dt = 0.01;
t_data = 0:dt:tf;
Y0 = [S0; I0; R0];
M = 1000;
alpha = 0.2;
beta = 15;
A = rand(M,4);
A(:,2) = betarnd(alpha,beta,M,1);

ode_options = odeset('RelTol',1e-6);
for j=1:M
    params = A(j,:);
    [t,Y] = ode45(@SIR_rhs,t_data,Y0,ode_options,params);
    y_A(j) = sum(dt*Y(:,3));
end
```

The associated function is

```
%
%           SIR_rhs
```

```
%
  function dy = SIR_rhs(t,y,params);

  N = 1000;

  gamma = params(1);
  k = params(2);
  r = params(3);
  mu = params(4);

  dy = [mu*N - mu*y(1) - gamma*k*y(2)*y(1);
        gamma*k*y(2)*y(1) - (r + mu)*y(2);
        r*y(2) - mu*y(3)];
```