Math 540: Project 3

Due Tuesday, March 3

1. Exercise 7.7 in the text or Exercise 14.2 in the new chapter. You should use the sensitivity relations $\frac{\partial y}{\partial \Phi}$ and $\frac{\partial y}{\partial h}$, which you computed in Problem 1 of Project 2, to construct your covariance matrix. You can also use the code posted at the book website for Exercise 7.16.

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 on the interval $[0, 0.8]$ and $q = [\alpha_1, \alpha_{11}, \alpha_{111}]$ are parameters. As in Project 2, we will employ the nominal values $\alpha_1 = -389.4, \alpha_{11} = 761.3$ and $\alpha_{111} = 61.5$.

(a) For $n = 81, 161$ and 801 equally spaced polarization values $P_i = (i-1)\Delta P, \Delta P = \frac{0.8}{n-1}, i = 1, \ldots, n$, compute the model response $\psi(P_i, q)$ and observations

$$\Upsilon_i = \psi(P_i, q) + \varepsilon_i,$$

where $\varepsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2)$ with $\sigma = 2.2$. In each case, compute the OLS estimate for the observation variance σ^2 and compare it to the true value. What do you observe?

(b) For $n = 161$, use the normal equations to approximate the parameters and compare to the nominal values. Compute the covariance matrix estimate V and discuss the correlation of the parameters. Discuss why global sensitivity methods, with the assumption of mutually independent parameters, may give misleading results as demonstrated in Project 2. Compute 95% confidence intervals and plot the residuals and the upper and lower confidence values in one figure. Do the intervals appear to be correct? Finally, plot the model and observations as a function of the polarization values.

3. Consider the SIR model

$$\begin{aligned}
\frac{dS}{dt} &= \delta N - \delta S - \gamma IS \quad , \quad S(0) = 900, \\
\frac{dI}{dt} &= \gamma IS - (r + \delta)I \quad , \quad I(0) = 100, \\
\frac{dR}{dt} &= rI - \delta R \quad , \quad R(0) = 0,
\end{aligned}$$

where γ, r and δ are each in the interval $[0, 1]$. The parameter vector is $q = [\gamma, r, \delta]$

(a) Use the data in the file `SIR.txt` to estimate the parameters q using the routine `fminsearch.m`. The first column contains times t_j and the second is corresponding values $I(t_j)$. You can approximate the solution to the ODE system using `ode45.m`, as you did in Project 2.

(b) Construct the local sensitivity matrix using complex-step, finite-differences or by formulating and numerically solving the sensitivity equations. Estimate the variance σ^2 of the observations, compute the covariance matrix V, and discuss the parameter correlation. Is V full rank and are your results to be expected.

(c) Using the parameter estimates and variances, use the command `normpdf.m` to plot the sampling distributions for each of the three parameters. Additionally, you should plot your residuals, your model fit to the data $I(t_j)$ and the trajectories for $S(t), I(t)$ and $R(t)$.