Math 540: Project 1

Tilekbek Zhoroev

1. Consider the spring model

$$\frac{d^2 z}{dt^2} + C\frac{dz}{dt} + Kz = 0$$
$$z(0) = 2, \quad \frac{d}{dt}z(0) = -C$$

with inputs $\Theta = [K, C]$. Use the complex-step approximation to compute the sensitivities $\frac{\partial z}{\partial K}$ and $\frac{\partial z}{\partial C}$ for $K = 20.5$ and $C = 1.5$ and compare with finite-difference approximations and the analytic values.

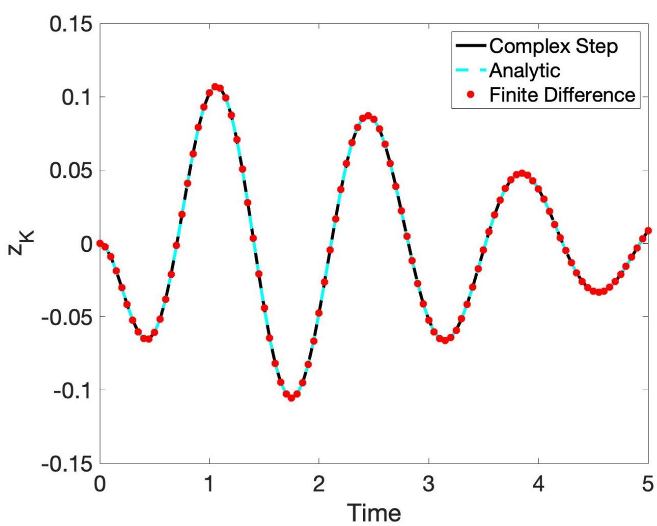
Solution. In textbook we have given the analytic solution of tge spring model as

$$y(t) = 2e^{-Ct/2}\cos(\sqrt{K - C^2/4}\,t)$$

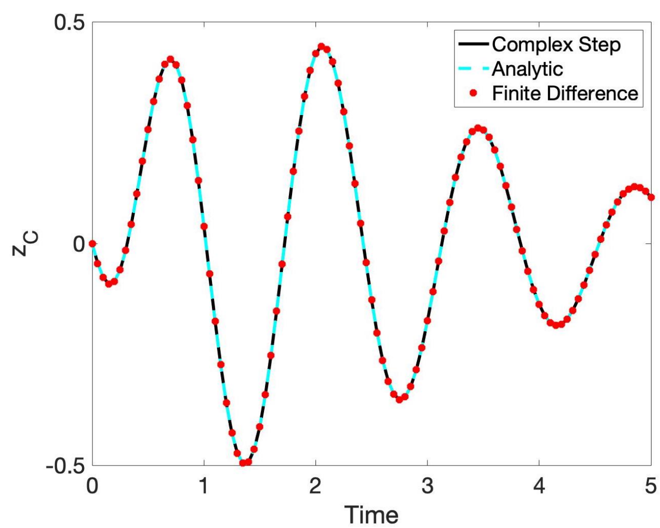
when $C^2 - 4K < 0$, and the local sensitivities are

$$\frac{dy}{dK} = e^{-Ct/2}\frac{-2t}{4K - C^2}\sin(\sqrt{K - C^2/4}\,t)$$
$$\frac{dy}{dC} = e^{-Ct/2}\left[\frac{Ct}{4K - C^2}\sin(\sqrt{K - C^2/4}\,t) - t\cos(\sqrt{K - C^2/4}\,t)\right].$$

For this problem we have given analytic solution, hence we would use this for the finite difference and complex step approximation, i.e.



(a)



(b)

Figure 1: Comparison of complex-step and finite difference approximations with analytic differentiation, (a) $\frac{\partial z}{\partial K}$; (b) $\frac{\partial z}{\partial C}$.

$$f'(x) \approx \frac{Im(f(x+ih))}{h}$$

and

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Here we choose $h = 10^{-8}$ for finite difference approximation and $h = 10^{-16}$. The comparison graphs are given in Figure 1 (a) and (b). We observe that both graphs both approximations are good for this problem. We can also analyse their convergence rates by changing h values on both approximations.

2. Apply the Parameter Subset Selection to the 4 parameter SIR model

$$\begin{aligned}
\frac{dS}{dt} &= \delta N - \delta S - \gamma k I S, & S(0) &= S_0 \\
\frac{dI}{dt} &= \gamma k I S - (r+\delta) I, & I(0) &= I_0 \\
\frac{dR}{dt} &= rI - \delta R, & R(0) &= R_0
\end{aligned}$$

detailed in Example 3.6. The initial conditions are $S_0 = 900, R_0 = 0$ and $I_0 = 100$ so $N = 1000$. You can take the recovered individuals $R(t_i)$ as your response, where $t_i \in [0, 5]$ are 50 equally-spaced time values. Using the nominal values $[0.2, 0.1, 0.15, 0.6]$ for the parameters $\Theta = [(\gamma, k, \delta, r]$, determine an identifiable parameter set.

Solution. In this problem we don't know the analytic solution of the system, so we would use the ode solvers, e.g **ode45.m**. Let us find the components of the sensitivity equations with respect to each parameter. Hence we have,

$$\mathbf{s}(t) = \left[\frac{\partial S}{\partial \gamma}, \frac{\partial I}{\partial \gamma}, \frac{\partial R}{\partial \gamma}, \frac{\partial S}{\partial k}, \frac{\partial I}{\partial k}, \frac{\partial R}{\partial k}, \frac{\partial S}{\partial \delta}, \frac{\partial I}{\partial \delta}, \frac{\partial R}{\partial \delta}, \frac{\partial S}{\partial r}, \frac{\partial I}{\partial r}, \frac{\partial R}{\partial r}\right]^\top$$

$$\frac{\partial \mathbf{g}}{\partial \mathbf{u}} = \begin{bmatrix} \mathbf{J} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{J} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{J} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{J} \end{bmatrix}$$

$$\mathbf{J} = \begin{bmatrix} -\delta - \gamma k I & -\gamma k S & 0 \\ \gamma k I & \gamma k S - (r+\delta) & 0 \\ 0 & r & -\delta \end{bmatrix}$$

$$\frac{\partial \mathbf{g}}{\partial \alpha} = \Big[-kIS,\ kIS,\ 0,\ -\gamma IS,\ \gamma IS,\ 0,\ N-S,\ -I,\ -R,\ 0,\ -I,\ I \Big]^\top$$

Then, putting all together,

$$\begin{aligned}
\frac{d\,\mathbf{s}(t)}{dt} &= \frac{\partial \mathbf{g}}{\partial \mathbf{u}} \mathbf{s}(t) + \frac{\partial \mathbf{g}}{\partial \alpha} \\
\mathbf{s}(0) &= \mathbf{0}_{12}
\end{aligned}$$

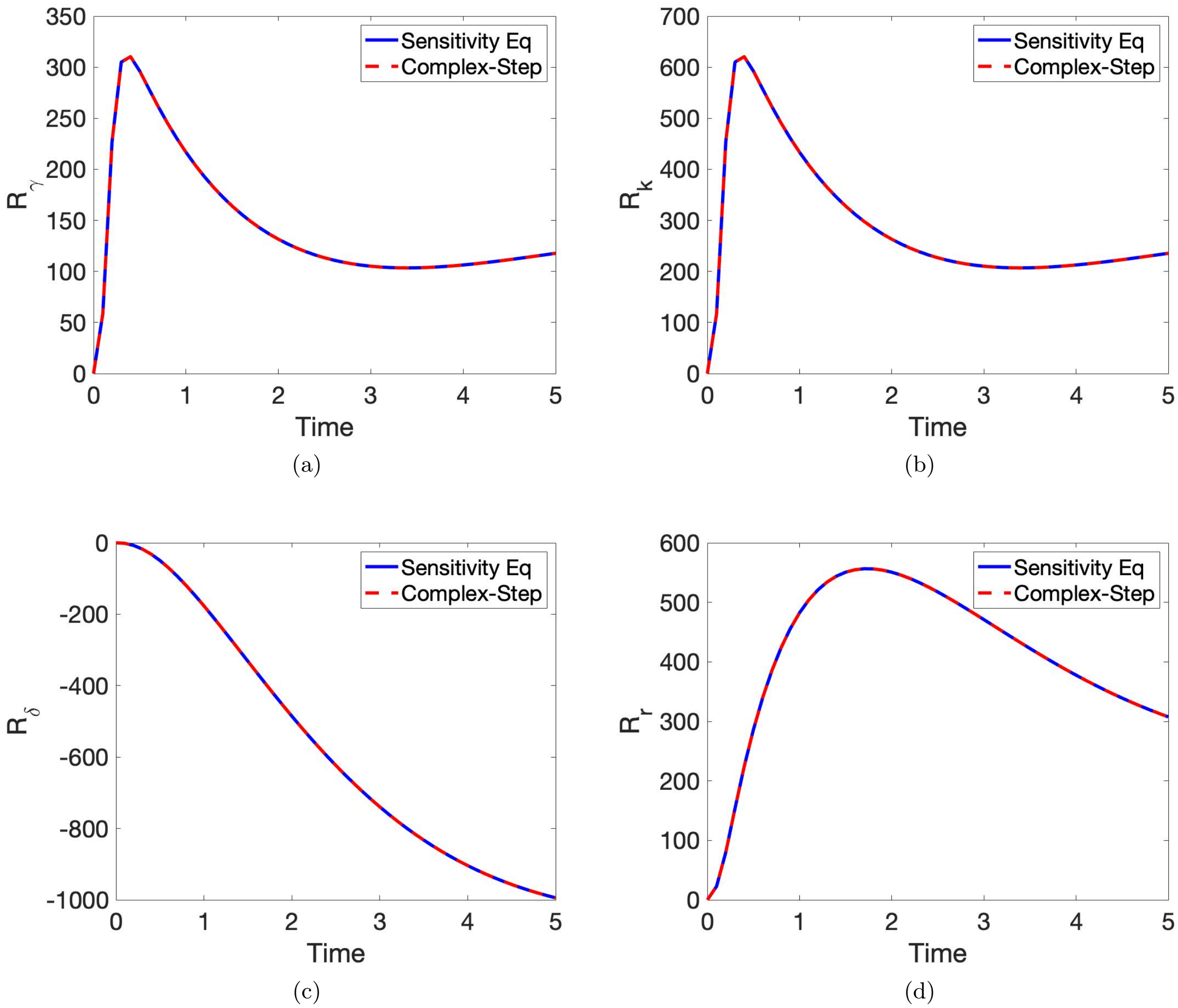


Figure 2: Sensitivity equations comparing results with complex-step approximations; (a) $\frac{\partial R(t)}{\partial \gamma}$; (b) $\frac{\partial R(t)}{\partial k}$; (c) $\frac{\partial R(t)}{\partial \delta}$; (d) $\frac{\partial R(t)}{\partial r}$

with given SIR model we obtain the solutions. Before applying parameter subset selection algorithm we want to verify the results of the sensitivity equations with the results using complex step approximations. The sensitivities of $R(t)$ with respect to each parameters are given in Figure 2 (a), (b), (c), and (d). Next, we construct our sensitivity matrix as

$$\mathbf{S} = \begin{bmatrix} \frac{\partial}{\partial\gamma}R(t_1) & \frac{\partial}{\partial k}R(t_1) & \frac{\partial}{\partial\delta}R(t_1) & \frac{\partial}{\partial r}R(t_1) \\ \frac{\partial}{\partial\gamma}R(t_2) & \frac{\partial}{\partial k}R(t_2) & \frac{\partial}{\partial\delta}R(t_2) & \frac{\partial}{\partial r}R(t_2) \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial}{\partial\gamma}R(t_{50}) & \frac{\partial}{\partial k}R(t_{50}) & \frac{\partial}{\partial\delta}R(t_{50}) & \frac{\partial}{\partial r}R(t_{50}) \end{bmatrix}.$$

Subsequently we applied parameter subset selection to the different η values and the results are presented in Table 1.

eta	***Identifiable parameters***	***Nonidentifiable parameters***
10^{-4}	$\{k, \delta, r\}$	$\{\gamma\}$
10^{-6}	$\{k, \delta, r\}$	$\{\gamma\}$
10^{-8}	$\{k, \delta, r\}$	$\{\gamma\}$
10^{-10}	$\{\gamma, k, \delta, r\}$	$\emptyset$

Table 1: Parameter Subset Selection results of SIR model

3. Consider

$$\begin{aligned} \frac{d^2 T_s(x)}{dx^2} &= \frac{2(a+b)h}{kab}[T_s(x) - T_{amb}], \quad 0 < x < L \\ \frac{dT_s}{dx}(0) &= \frac{\Phi}{k} \\ \frac{dT_s}{dx}(L) &= \frac{h}{k}[T_{amb} - T_s(L)]. \end{aligned}$$

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

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

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

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

The measured ambient room temperature is $T_{amb} = 21.29C$ and the rod has cross sectional dimensions $a = b = 0.95$ cm and length $L = 70cm$. You can employ the nominal parameter values $k = 2.37, h = 0.00191$ and $\Phi = -18.4$ which we infer through frequentest and Bayesian inference.

(a) Use finite-differences and complex-step derivative approximations to approximate the sensitivity relations $\frac{\partial f}{\partial \Phi}$, $\frac{\partial f}{\partial h}$ and $\frac{\partial f}{\partial k}$ and plot your solutions at the 15 equally spaced spatial locations $x_i = x_0 + (i-1)\Delta x$, where $x_0 = 10cm$ and $\Delta x = 4cm$. Verify your approximations by comparing with analytic sensitivity values.

(b) For the parameters $\Theta = [\Phi, h, k]$, construct the sensitivity matrix

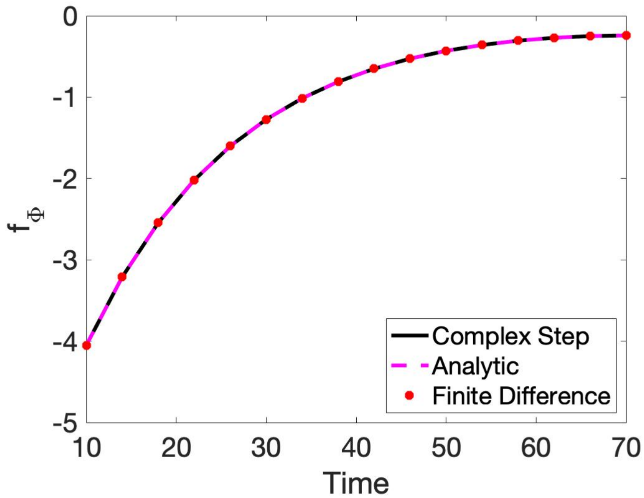
$$\mathbf{S}_{ij} = \frac{\partial f}{\partial \Theta_j}(x_i, \Theta)$$

and scaled Fisher information matrix $\mathbf{F} = \mathbf{S}^\top \mathbf{S}$. Compute the singular values of $\mathbf{S}$ and eigenvalues of $\mathbf{F}$ and discuss why your results are consistent with the model parameterization.

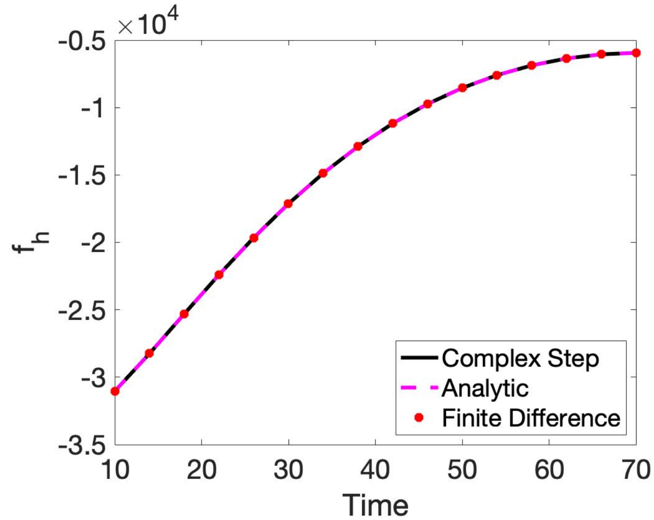
(c) As detailed in Example 3.8, the thermal conductivity k is well-documented for aluminum and copper. Fix this parameter and repeat your analysis for the parameters $\Theta = [\Phi, h]$. Are they identifiable?

Solution

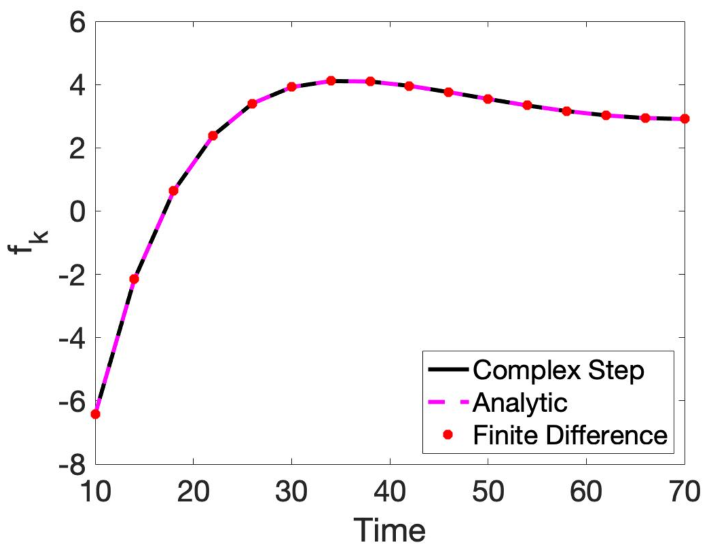
(a) By applying finite difference and complex step approximations to the analytic solution we obtain approximate sensitivity equations. Then we compare this results with analytic sensitivity values and the graph of comparisons are given in Figure 3 (a), (b), and (c).



(a)



(b)



(c)

Figure 3: Comparison of complex-step and finite difference approximations with analytic differentiation, (a) $\frac{\partial f}{\partial \Phi}$; (b) $\frac{\partial z}{\partial h}$; (c) $\frac{\partial z}{\partial k}$.

(b) Using given formula of the sensitivity matrix we constructed it and the we obtain singular values of it,

$$\left\{6.6945 \times 10^4,\ 1.3758 \times 10^1,\ 2.8262 \times 10^{-13}\right\}$$

and eigenvalues of Fisher information matrix,

$$\left\{4.4817 \times 10^9,\ 1.8927 \times 10^2,\ 3.5947 \times 10^{-14}\right\}$$

Using eigenvalues we observe that one eigenvalue is near to zero, hence let us check eigenvector corresponds to this eigenvalue to identify least influential parameter. The eigenvector is,

$$\left[9.9181 \times 10^{-1},\ -1.0295 \times 10^{-4},\ -1.2775 \times 10^{-1},\right]^\top$$

and we conclude that Φ is unidentifiable parameter. This is consistent with the model parameterization, since we have given parameters are given in form of $\frac{\Phi}{k}$ or $\frac{h}{k}$. One can obtain their ratio uniquely but not both of them simultaneously.

(c) Using this two parameter we obtain sensitivity matrix and it's singular values are,

$$\left\{6.6945 \times 10^4,\ 1.7575\right\}$$

and eigenvalues of Fisher matrix,

$$\left\{4.4817 \times 10^9,\ 3.0888\right\}.$$

Since eigenvalues are not small we conclude that both parameters are identifiable.

4. Consider the Helmholtz energy

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

where P is the polarization and $\theta = [\alpha_1, \alpha_{11}, \alpha_{111}]$ 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 $U(0, 1)$ and map to the interval $[\alpha_l, \alpha_r]$ that is 20% above and below the nominal value. For uniformly sampling on the interval $[a, b]$, one would use the MATLAB command $\theta = \mathbf{a} + (\mathbf{b} - \mathbf{a}) * \mathbf{rand(1, 1)}$.

(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 S and matrix $F = S^T S$ using 17 equally spaced polarization values in the domain $[0, 0.8]$. Compute the eigenvalues of F and discuss the identifiability of the parameters θ as specified by Algorithm 8.19. You can compare your results to Example 8.20.

(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

$$y(\theta) = \int_0^{0.8} \psi(P, \theta)\, dP$$

which you can compute analytically. To check your solution, show that $\mu^* \approx \left[\frac{\partial y}{\partial \alpha_1}, \frac{\partial y}{\partial \alpha_{11}}, \frac{\partial y}{\partial \alpha_{111}}\right]$. Which parameter is least influential?

(d) Use the Saltelli Algorithm 9.8 to approximate the Sobol sensitivity indices S_i and S_{T_i}. Compare your values of S_i to the analytic values reported in Example 9.12 and 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 Algorithm 9.8. 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.

Solution

(a) Using nominal values of the parameters and P in the the interval $[-0.8,\ 0.8]$ we obtained the plot of the Helmholtz energy. The graph is given in Figure 4 and we observe that the double-well behavior.

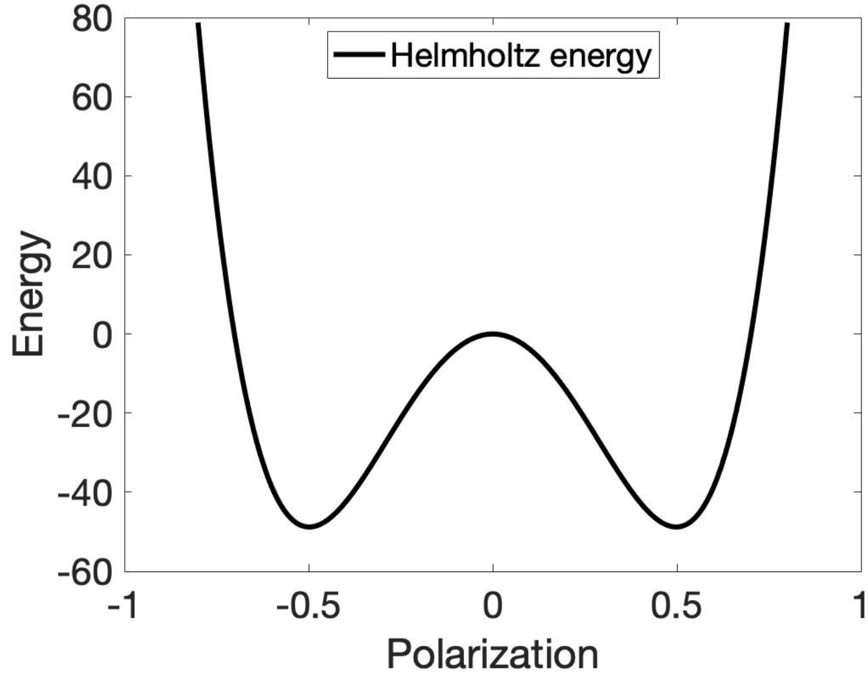


Figure 4: The graph of the Helmholtz energy

(b) Using equation of the energy function we obtain sensitivity matrix,

$$\begin{aligned}\mathbf{S} &= \Big[\frac{\partial\psi}{\partial\alpha_1},\ \frac{\partial\psi}{\partial\alpha_{11}},\ \frac{\partial\psi}{\partial\alpha_{111}}\Big]\\ &= \Big[P^2,\ P^4,\ P^6\Big].\end{aligned}$$

then the eigenvalues are

$$\Big\{0.0004, 0.0425, 1.9934\Big\}.$$

If we take $\eta < 0.0004$ then all parameters are identifiable. But the we can find the least identifiable parameter using eigenvector of Fisher matrix corresponding to smallest eigenvalue,

$$\Big[-0.1249,\ 0.6519,\ -0.7479\Big]^\top$$

and we conclude that α_{111} is least identifiable parameter.

(c) Let us compute the scalar response analytically,

$$\begin{aligned}y(\theta) &= \int_0^{0.8} \psi(P,\theta)\,dP\\ &= \alpha_1\frac{0.8^3}{3} + \alpha_{11}\frac{0.8^5}{5} + \alpha_{111}\frac{0.8^7}{7}.\end{aligned}$$

Then we apply Morris screening to this response. In each iteration we get sample parameters from uniform distribution from $\pm 20\%$ of the nominal values and we applied forward difference to the response respect to each parameter. Finally the we obtain

$$\mu^* = \big[0.1707,\ 0.0655,\ 0.03\big]$$

and

$$\sigma^2 = \left[0.1244 \times 10^{-25},\, 0.0778 \times 10^{-25},\, 0.0012 \times 10^{-25}\right]$$

after comparing results we conclude that α_{111} is least identifiable parameter and this results is consistent with part (b). Moreover we observe that,

$$\begin{aligned} \mu^* &= [0.1707,\, 0.0655,\, 0.03] \\ &\approx \left[\frac{0.8^3}{3}, \frac{0.8^5}{5}, \frac{0.8^7}{7}\right] \\ &= \left[\frac{\partial y}{\partial \alpha_1}, \frac{\partial y}{\partial \alpha_{11}}, \frac{\partial y}{\partial \alpha_{111}}\right]. \end{aligned}$$

(d) Using Saltelli Algorithm with $M = 10^4$ we obtain approximate Sobol sensitive indices

$$\mathbf{S} = \left[0.6384,\, 0.3598,\, 4.2568 \times 10^{-4}\right]$$

and

$$\mathbf{S}_T = \left[0.6395,\, 0.3606,\, 4.9117 \times 10^{-4}\right].$$

This results are approximately same as analytic values and

$$S_1 + S_2 + S_3 = 0.9987 \approx 1$$

as desired.It implies that higher order interactions S_{ij} are negligible. Moreover, since S_3 is small we infer that α_{111} is noninfluential parameter.

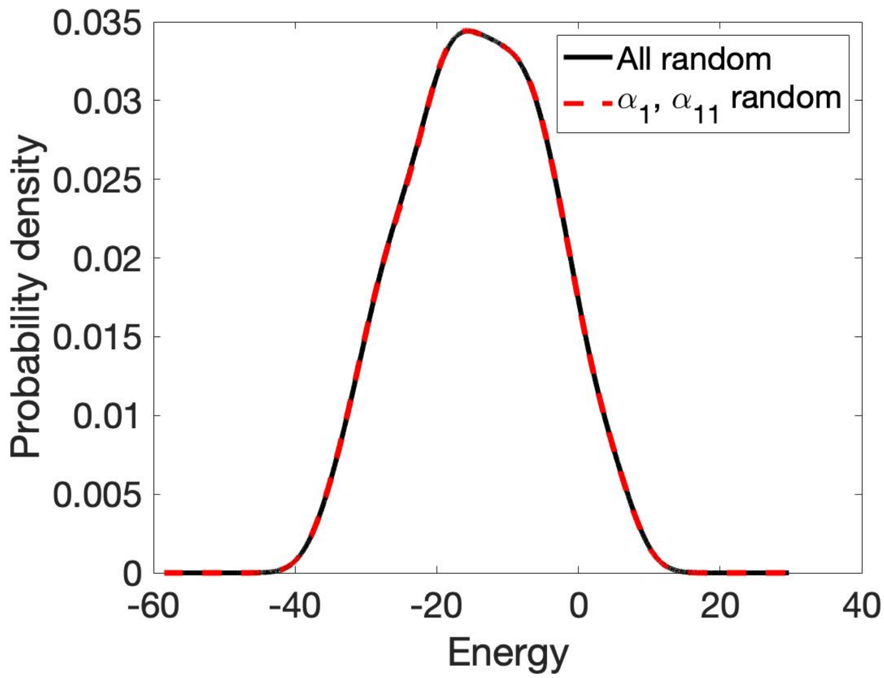


Figure 5: Distributions of y

Next we obtain the PDF of response for all random parameters and random parameters except noninfluential parameters, their plots are given in Figure 5. We observe that both of the PDF are similar to each other. In part (b) all parameters were identifiable for small η values and it's not consistent with this result.