

In the name of God

Department of Physics Shahid Beheshti University

ADVANCED COURSE ON COMPUTATIONAL PHYSICS

Exercise Set 14

(Due Date: 1403/10/20)

1. Fisher matrix for a differential equation: Suppose that the theoretical prediction is given by following equation:

$$\frac{d^2 G}{d \ln^2 x} + \frac{3}{2} \left(\frac{1}{3} + \frac{\Omega_k(x)}{2} - w(x)\Omega_\lambda(x) \right) \frac{dG}{d \ln x} - \frac{3}{2} \Omega_m(x)G = 0$$

here $\Omega_k(x) = [1 - (\Omega_m + \Omega_\lambda)]/x^2$, $\Omega_m(x) = \frac{\Omega_m x^{-3}}{[\Omega_m x^{-3} + \Omega_\lambda x^{-3(1+w(x))} - \Omega_k x^{-2}]}$, $\Omega_\lambda(x) = \frac{\Omega_\lambda x^{-3(1+w(x))}}{[\Omega_m x^{-3} + \Omega_\lambda x^{-3(1+w(x))} - \Omega_k x^{-2}]}$ and $\Omega_k = [1 - (\Omega_m + \Omega_\lambda)]$ and $w(x) = w_0 + w_1 x$. The parameter is $\{\Theta\} \equiv \{\Omega_m = 0.27, \Omega_\lambda = 0.73, H_0 = 70, w_0 = -1, w_1 = 0.1\}$. Now taking into account the x.txt series containing the $\{x\}$ values and COV.txt as the covariance of systematic errors, determine the contours for 1σ , 2σ and 3σ for each pairs of parameter in addition to one-dimensional likelihood analysis.

2. Fisher matrix to asses the interaction between Ar molecules. Suppose that in a thought experiment, we measure the internal energy of Ar for different temperature. The theoretical internal energy per number of particel is given by:

$$E(T) = \frac{3k_B T}{2} + \frac{n}{2} \int u(r)g(r)d^3r$$

here $u(r) = 4\epsilon \left[\left(\frac{a}{r} \right)^a - \left(\frac{b}{r} \right)^b \right]$ and the pair correlation is $g(r) = e^{-\beta u(r) + \beta n F(r)}$ with $F = q\beta$, $\beta = k_B T$. If the model parameters are $\{\Theta\} = \{a = 12, b = 6, \epsilon = 0.997 kJ/mol, \alpha = 3.40 A^\circ, \sigma = 3.45 A^\circ, q = 0.001\}$. Suppose that we have one mole ($n = 1$). Now taking into account the x.txt series containing the $\{x\}$ values and COV.txt as the covariance of systematic errors, determine the contours for 1σ , 2σ and 3σ for each pairs of parameter in addition to one-dimensional likelihood analysis. (You can use any other physical assumptions that you think they can be useful)

3. According to the simple Genetic Algorithm and considering the $y_{theory} = ax^H$ compute a and H for *data-exp2.txt*. Compare your results with those determined by MCMC and HMC done in previous question.

Good luck, Movahed
