Math 540: Project 3

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1. Use the posted MATLAB code to repeat the analysis in Example 12.17 for the copper rod data in Table 3.7. You should use the value $k = 4.01$ for the thermal conductivity of copper and the ambient air temperature $u_{amb} = 22.28$. Compare the chains and marginal distributions computed using the Metropolis Algorithm 12.9 with those generated by DRAM. Compare your results with the frequentist estimates computed in Exercise 11.5.

   Solution.

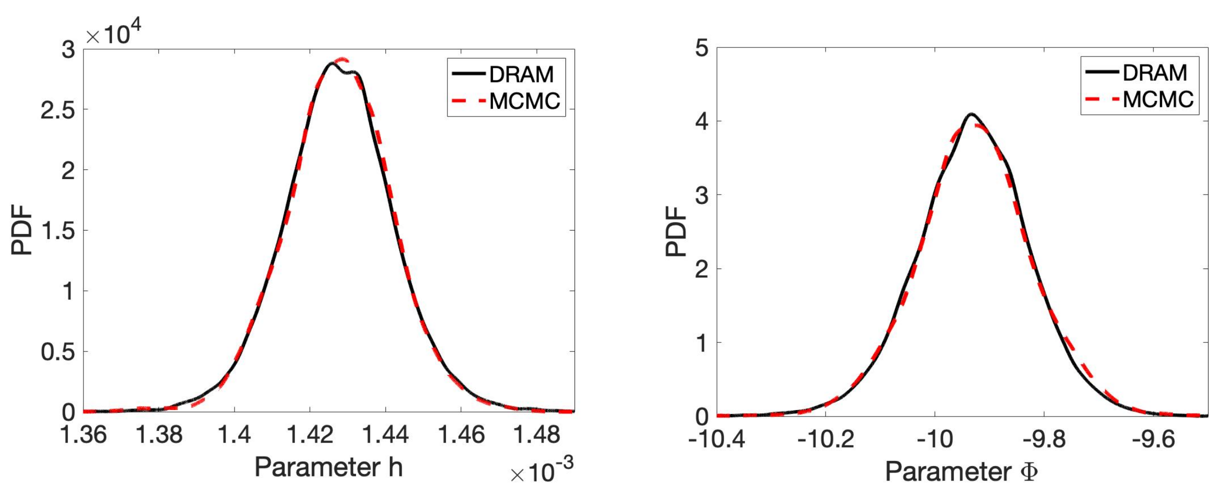
   In previous project, we obtained the optimal parameter values using Frequentist approach. More information about data and model are presented in Project 1 and 2. Here to apply Metropolis Algorithm we used the covariance matrix,

$$\mathbf{V} = \begin{bmatrix} 0.0090 & -1.2117 \times 10^{-6} \\ -1.2117 \times 10^{-6} & 1.7726 \times 10^{-10} \end{bmatrix} \tag{1}$$

   which is obtained by using optimal parameters. As described in Metropolis Algorithm 12.9 we used the $R = \mathbf{col}(\mathbf{V})$, to define the proposal distribution. To get faster convergence in MCMC we choose the initial values of the parameters, the optimal parameters obtained by Frequentist approach, $\Phi = -9.9265$ and $h = 0.0014$. The trace plots of the MCMC algorithm for each parameter are given in Figure 2 (a) and (b) and joint sample points are presented in Figure 2 (c). The error variance at each iteration is presented in Figure 2 (g). Here the acceptance probability is

$$P(accept\ \theta^*) = 0.2701.$$

   Next, we would like analyse same model using DRAM algorithm. For this algorithm we used same initial value and same covariance matrix. The chain plots, scatter plot of the joints samples, and error variances are given in Figure 2 {(d), (e) }, (f), and (h), respectively. By



(a) (b)

Figure 1: The marginal posterior distributions of the parameter (a) h and (b) Φ using DRAM and MCMC.

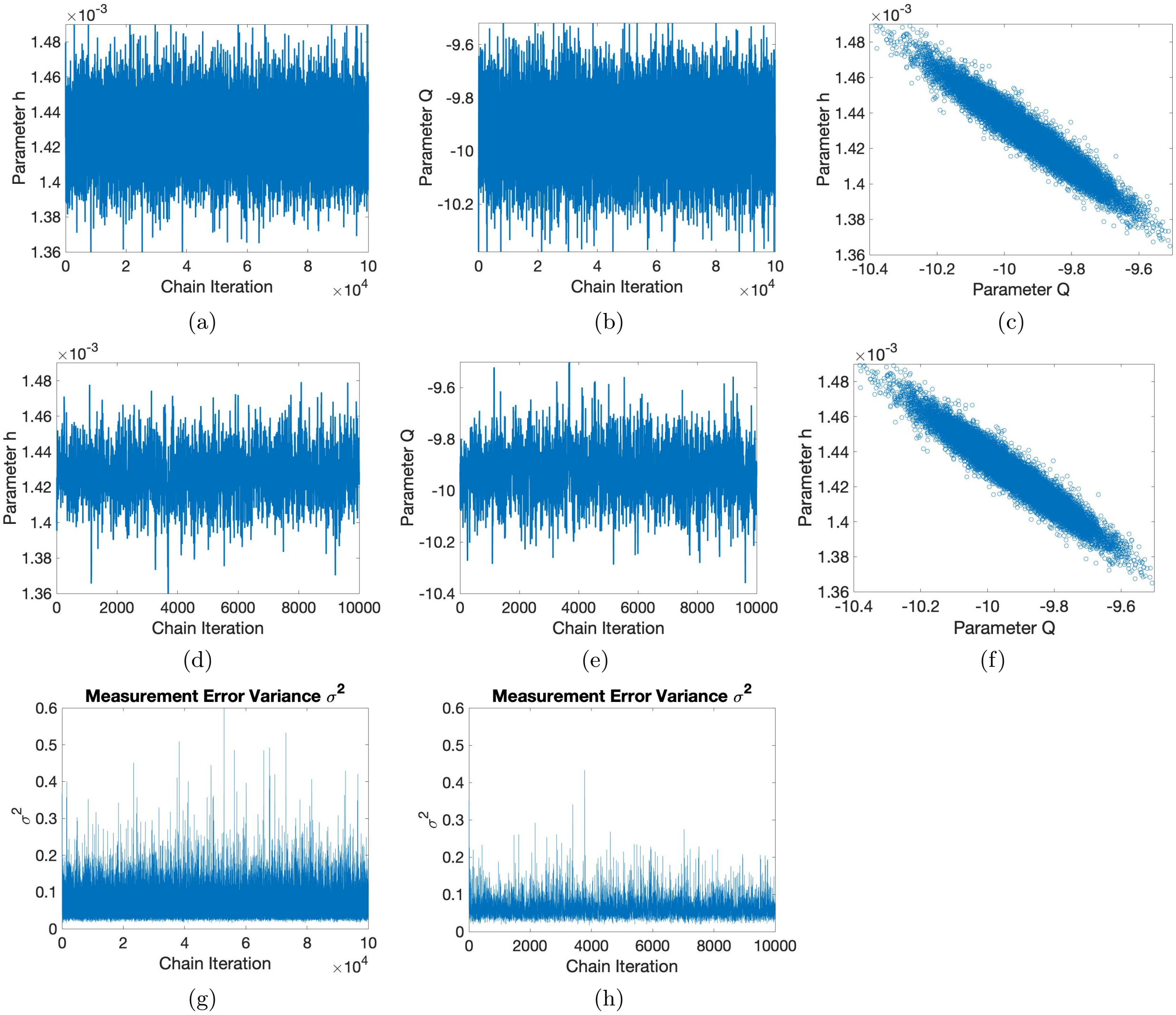


Figure 2: The plots of the chain and joints samples using DRAM and Metropolis Algorithm.

comparing two graphs of two algorithm we observe that the samples obtained through DRAM algorithm is closer to center and variances are also smaller than chain obtained by MCMC algorithm. The marginal posterior distributions of the each parameters obtained by both algorithms are presented in Figure 1. From graph we observe that the posterior distributions are very close to each other. Next, we would like to compare the covariance matrix of the chain and initial covariance matrix. The chain covariance matrix using DRAM algorithm is

$$\mathbf{V} = \begin{bmatrix} 0.01127 & -1.5201 \times 10^{-6} \\ -1.5201 \times 10^{-6} & 2.2261 \times 10^{-10} \end{bmatrix}$$

and it's very close to initial covariance in (1) (Frequentist approximation of the covariance matrix). From Table 1, we observe that the parameter estimations using each each algorithms are close to each other. The standard deviations of the observation error and parameter are represented in Table 1. The standard deviations obtained by Bayesian approach is bigger than Frequentist estimation.

	h	Φ	σ	σ_h	σ_Φ
OLS	0.0014	-9.9265	0.2301	0.0947	1.3314×10^{-5}
MCMC	0.0014	-9.9281	0.2542	0.0105	1.4716×10^{-5}
DRAM	0.0014	-9.9285	0.2556	0.0106	1.49200×10^{-5}

Table 1: The parameter estimations and standard deviations using OLS, MCMC and DRAM algorithms

2. Consider the following SIR model,

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

where γ, r and δ are each in the interval [0, 1]. We will revisit this problem in Exercise 13.5 to construct Bayesian credible and prediction intervals for each of the states.

(a) The file **SIR.txt** contains times t_j in the first column and corresponding values $I(t_j)$ in the second, and the parameters $\boldsymbol{\theta} = [\gamma, r, \delta]$. Employ DRAM to compute and plot chains, marginal densities, and pairwise plots for the parameters. You should use **s2chain** to additionally estimate the observations variance σ^2. You can use the covariance matrix $\mathbf{V}$, which you estimated in Exercise 11.7, as input. How do the mean parameter values compare to the OLS estimates that you computed using **fminsearch.m**? How does the final adapted covariance matrix compare to your initial estimate $\mathbf{V}$? Plot the marginal densities and OLS distributions in the same figures and discuss your results. Finally, how does the variance estimate σ^2 computed by DRAM compare to your OLS estimate?

(b) Now consider the model

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

non-identifiable parameter set $\boldsymbol{\theta} = [\gamma, r, \delta, k]$. Run DRAM and plot the pairwise distributions. Are your chains converging? Can you use the Bayesian analysis to establish which parameters are not mutually identifiable?

(c) As noted in Exercise 11.7(d), it is appropriate to specify $\delta = 0$ in the SIR model (12.38) due to the short duration of the outbreak. Furthermore, you can take $S(0) = 760$, $I(0) = 3$ and $R(0) = 0$ so that $N = 763$. Use DRAM to construct posterior distributions for $\boldsymbol{\theta} = [\gamma, r]$.. How do your mean parameter values compare to the OLS estimates obtained in Exercise 11.7(d)?

Solution.

(a) The estimated parameters by OLS,

$$\gamma = 0.0100,\ \delta = 0.1953,\ r = 0.7970$$

are employed as an initial value to the DRAM algorithm. Moreover, the initial covariance matrix is,

$$\mathbf{V} = \begin{bmatrix} 1.7357 \times 10^{-8} & 1.8575 \times 10^{-7} & 1.4540 \times 10^{-7} \\ 1.8575 \times 10^{-7} & 2.6153 \times 10^{-5} & 3.1790 \times 10^{-5} \\ 1.4540 \times 10^{-7} & 3.1790 \times 10^{-5} & 8.4797 \times 10^{-5} \end{bmatrix}.$$

Then by this initial values and given data **SIR.txt**, we used the DRAM algorithm. The chain plots of each parameter, pairwise sample plots, and chains error variance are presented in Figure 3. From this plots we observe that the MCMC algorithm is converged. The estimated observational standard deviation is $\sigma = 21.0528$ and estimated standard

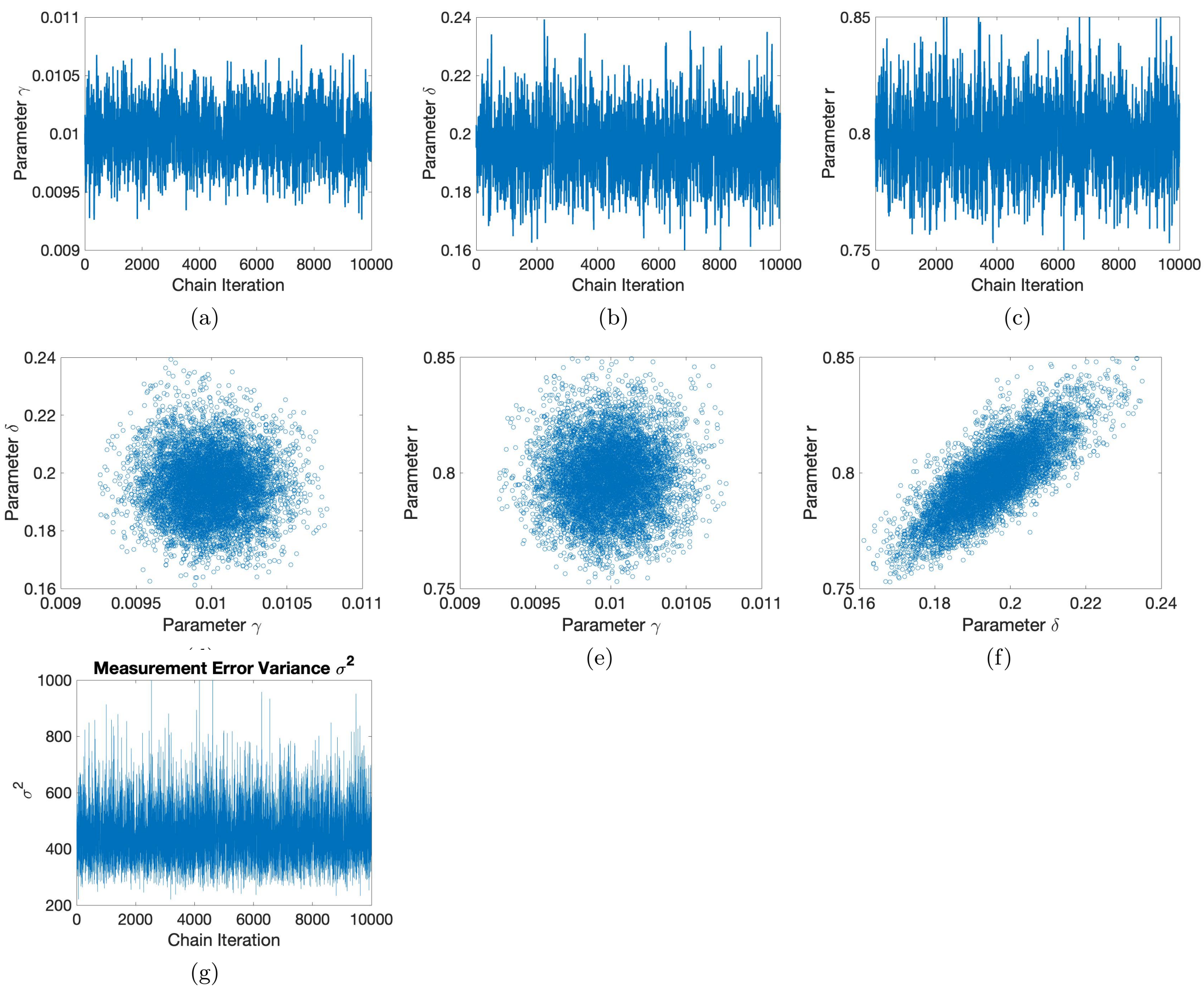
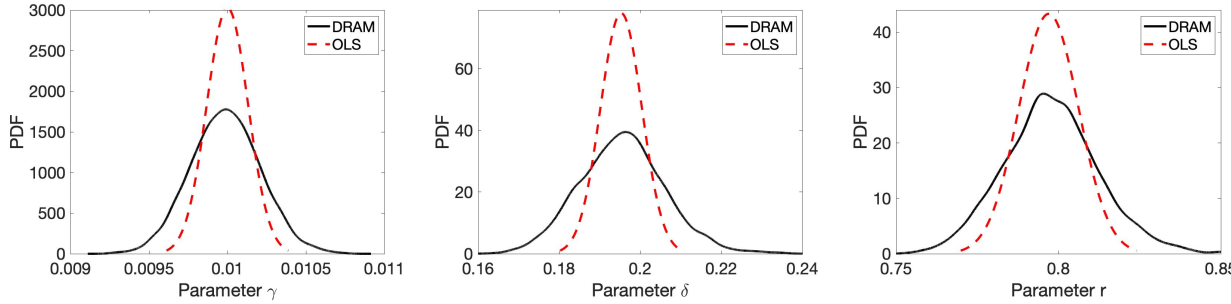


Figure 3: The plots of the chain and pairwise joints samples using DRAM algorithm.



(a) (b) (c)

Figure 4: The marginal posterior distributions of the parameter (a) γ, (b) δ, and (c) r using DRAM and OLS.

error using OLS was $\sigma = 20.6586$. The variance of the chain is,

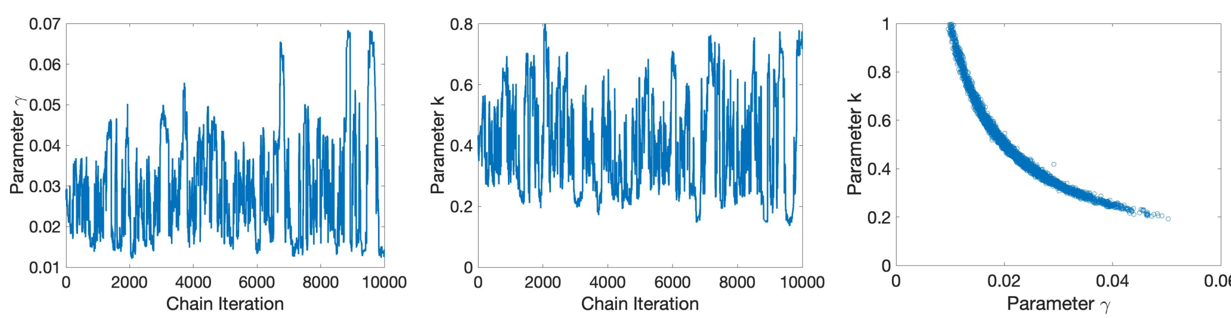
$$\mathbf{V} = \begin{bmatrix} 4.9214 \times 10^{-8} & 8.2561 \times 10^{-8} & 1.3512 \times 10^{-7} \\ 8.2561 \times 10^{-8} & 1.0218 \times 10^{-4} & 1.1635 \times 10^{-4} \\ 1.3512 \times 10^{-7} & 1.1635 \times 10^{-4} & 2.1544 \times 10^{-4} \end{bmatrix}$$

and it's different than initial covariance matrix. Hence, the distributions of the each parameter obtained by DRAM and OLS are different. The parameter estimations using Bayesian approach is

$$\gamma = 0.0100, \;\; \delta = 0.1958, \;\; r = 0.7979$$

and these are close to parameter estimations by Frequentist approach.

(b) Since we know that the all parameters are not identifiable, we specify random initial value to the parameter. Without specifying the initial covariance matrix we obtained the not converged chain. Trace plot for some parameters are given in Figure 5 (a) and (b). Next, we obtain the graph of the joint sample distribution in Figure 5 (c). From here we observe that $\gamma * k$ is equal to some number. Since the we have unidentifiable parameters we get this results. This shows that one can identify the mutually unidentifiable parameters using Bayesian analysis.



(a) (b) (c)

Figure 5: Trace plot of the MCMC for parameter (a) γ and (b) k; The joint sample of the parameter $gamma$ and k.

(c) In this case the initial parameters of of the DRAM algorithm are the estimated parameters using OLS,

$$\gamma = 0.0022, \ r = 0.4469$$

and covariance matrix

$$\mathbf{V} = \begin{bmatrix} 3.3117 \times 10^{-10} & 1.3030 \times 10^{-7} \\ 1.3030 \times 10^{-7} & 1.5355 \times 10^{-4} \end{bmatrix}.$$

The chain results are presented in Figure 6 (a), (b), and (c). From figure we observe that chain is converged. The marginal posterior distributions of each parameter is also given in Figure 6 (e), (f) and the distributions are looks normally distributed. The estimated parameters by Bayesian approach are

$$\gamma = 0.0022, \ r = 0.4487$$

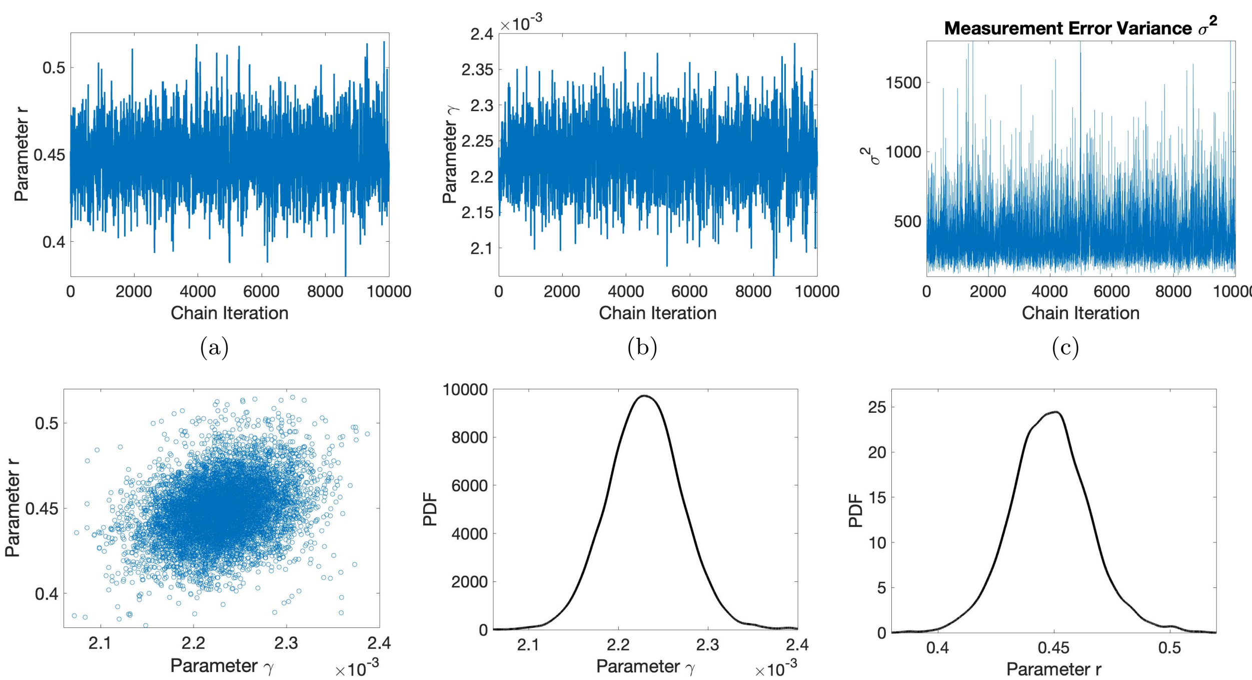
and this is almost same as OLS results. The estimations of the observational variance using Bayesian and Frequentist approach are

$$\sigma = 19.6142 \quad \text{and} \quad \sigma = 18.0413,$$

respectively. Finally, the covariance matrix of the chain is

$$\mathbf{V} = \begin{bmatrix} 1.9002 \times 10^{-9} & 2.3783 \times 10^{-7} \\ 2.3783 \times 10^{-7} & 2.8680 \times 10^{-4} \end{bmatrix}$$

and it has some differences from initial covariance matrix.



(a) (b) (c)

(d) (e) (f)

Figure 6: The plots of the chain and joints samples using DRAM.

3. Consider the Helmholtz energy

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

where P is the polarization on the interval $[0, 0.8]$ and $\boldsymbol{\theta} = [\alpha_1, \alpha_{11}, \alpha_{111}]^\top$ are parameters.We will revisit this problem in Exercise 13.6 to construct Bayesian credible and prediction intervals for responses.

(a) Using the data in the file **Helmholtz.txt**, which contains polarization values P_j in the first column and energies $\psi(P_j)$ in the second, employ DRAM to compute chains, marginal densities, and pairwise plots for the parameters. Report your parameter estimates and observation variance σ^2. Discuss the correlation of the parameters and why certain global sensitivity analysis techniques are not applicable.

(b) Now repeat (a) using the Random Walk Metropolis Algorithm 12.9. How do these results compare to DRAM?

Solution.

At the beginning we would like to approximate the parameters of the Helmholtz energy model using given data and **fminsearch.m.** The estimated parameter values are

$$\alpha_1 = -382.99, \alpha_{11} = 717.90, \alpha_{111} = 145.27.$$

Here we have $n = 81$ data points and $p = 3$ parameter, so the estimated observational error variance become

$$\sigma^2 = \frac{1}{n-p} \boldsymbol{R}^\top \boldsymbol{R} = 12.2068$$

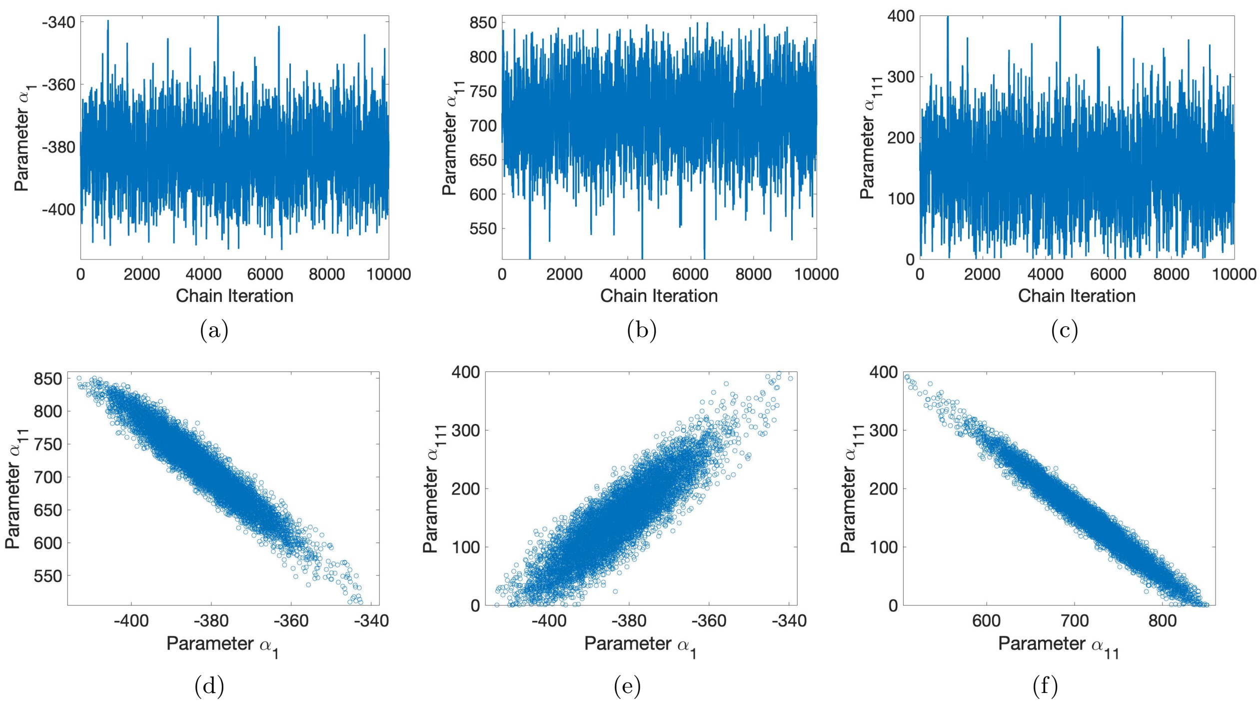
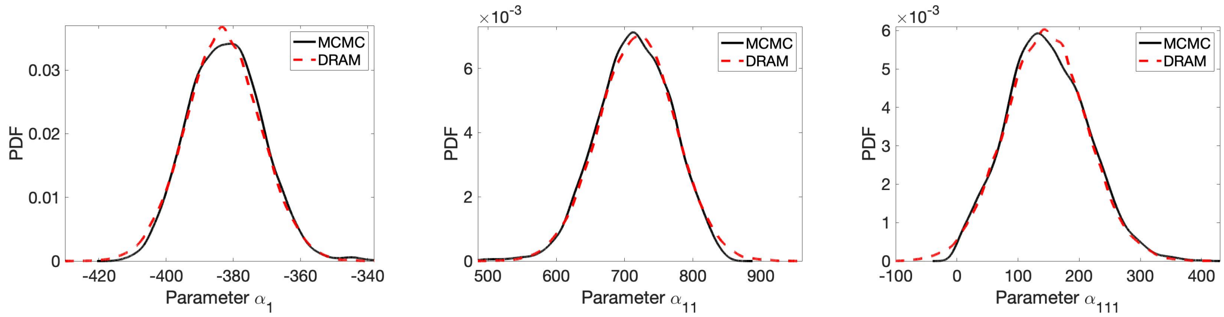


Figure 7: The plots of the chain and joints samples using DRAM.



(a) (b) (c)

Figure 8: The marginal posterior distributions of the parameter (a) α_1, (b)α_{11}, and (c) α_{111} Φ using DRAM and MCMC.

where $\boldsymbol{R}$ is the vector of residuals. Then the estimated covariance matrix become,

$$\mathbf{V} = \begin{bmatrix} 120.01 & -582.35 & 649.33 \\ -582.35 & 3.08 & -3.61 \\ 649.33 & -3.61 & 4.38 \end{bmatrix}.$$

We would use all this as an input for the DRAM algorithm. The chain results obtained by DRAM is presented in Figure 7 and Metropolis algorithm results given in Figure 9. In both cases the algorithm is converged and the results are close to each other. We observe that the marginal posterior distribution of each parameter obtained by DRAM and Metropolis algorithm, in Figure 8, are close to each other. Moreover the estimated parameters by DRAM algorithm is

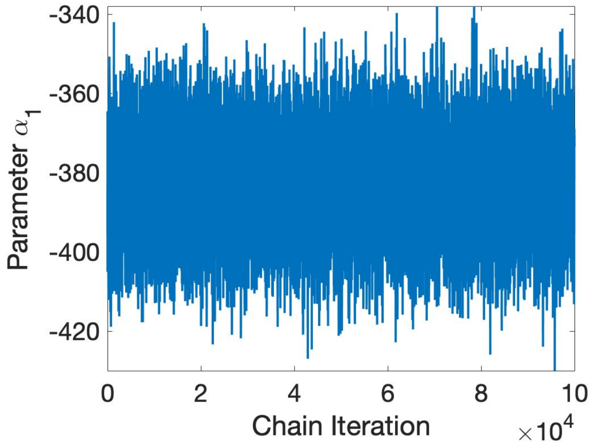
$$\alpha_1 = -382.47, \alpha_{11} = 715.6, \alpha_{111} = 147.88$$

and by Metropolis algorithm is

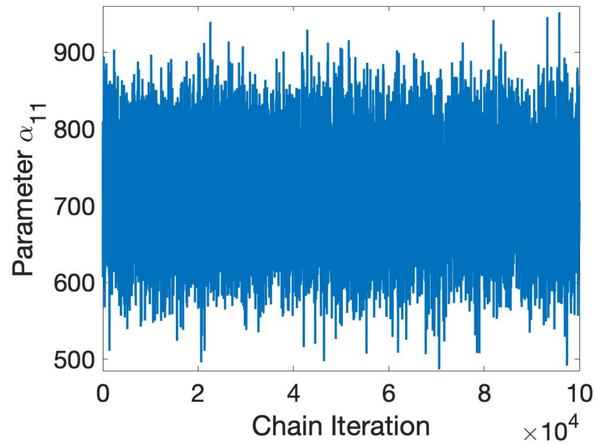
$$\alpha_1 = -382.87, \alpha_{11} = 716.99, \alpha_{111} = 146.48$$

and all the results are similar to each other. The estimated observational error variances using DRAM, Metropolis are $\sigma^2 = 13.4016$ and $\sigma^2 = 13.4187$, respectively. The estimated parameters are also close to OLS estimate. Finally, the covariance matrix of the chain of DRAM algorithm is

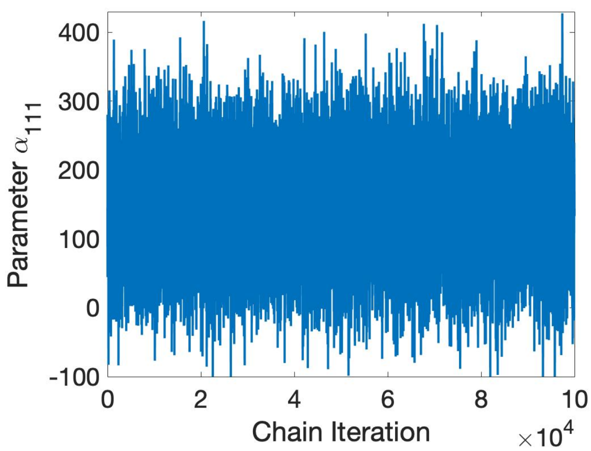
$$\mathbf{V} = \begin{bmatrix} 111.70 & -532.36 & 588.08 \\ -532.36 & 2.81 & -3.29 \\ 588.08 & -3.29 & 4.01 \end{bmatrix}.$$



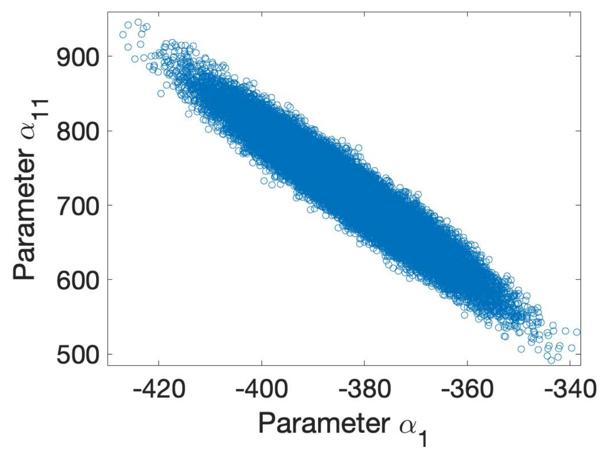
(a)



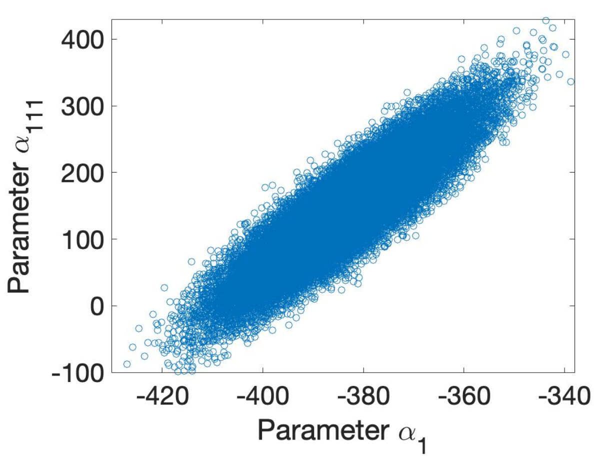
(b)



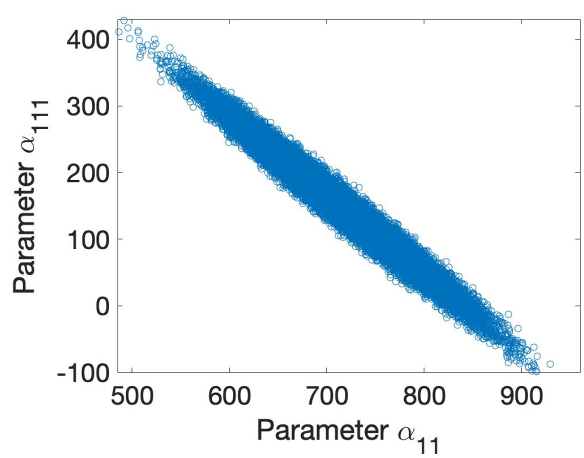
(c)



(d)



(e)



(f)

Figure 9: The plots of the chain and joints samples using Metropolis Algorithm.