Uncertain quantification for heat transfer in turbulent flow
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1 Introduction

In this project, we consider studying the estimation of coefficients of the Dittus-Boelter equation from empirical data with uncertainty quantification [4]. The Dittus-Boelter equation can be used to understand heat transfer for turbulent flow in circular tubes [5]. The equation allows the computation of the Nusselt number Nu from the Reynolds number Re and the Prandtl number Pr [2]. Nu is the ratio of convection to pure conduction heat transfer and measures local convection heat transfer at the boundary. Pr is the ratio of the momentum diffusivity to the thermal diffusivity. Re is the ratio of inertia to viscosity forces such that large values of Re represent turbulent flow [3]. For the case where the fluid is heating, the Dittus-Boelter equation

$$Nu = 0.023 Re^{0.8} Pr^{0.4}, \tag{1}$$

holds where $0.7 \leq Pr \leq 16,700$ and $Re \geq 10,000$, indicating turbulent flow [2]. The validity of equation (1) with coefficients $\boldsymbol{\theta} = [0.023, 0.8.0.4]$ has been verified empirically for these conditions. The leading coefficient was originally reported at values close to 0.023 by fitting to data [5]. We revisit the problem of determining the coefficients of the Dittus-Boelter equation (1) using the `db_data.txt` set of 56 empirical observations. However, we use the Bayesian framework for parameter estimation, treating $\boldsymbol{\theta}$ as a random variable. We first perform statistical identifiability analysis by constructing the Fisher information matrix. We then perform Bayesian inference to construct a distribution for $\boldsymbol{\theta}$ and compare to the results from identifiability analysis.

2 Identifiability

We analyze the identifiability of the parameters $\boldsymbol{\theta}$ with respect to the `db_data.txt` data set. A parameter is identifiable if we can uniquely determine its value from the data. In particular, we are interested in the statistical identifiability of the parameters in the observation model

$$Nu_i = \theta_1 Re_i^{\theta_2} Pr_i^{\theta_3} + \epsilon_i, \tag{2}$$

where Nu_i, Re_i, and Pr_i are the observed measurements of the Nusselt, Reynolds, and Prandtl numbers. Furthermore, $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ are errors in measurements, assumed to be identically and independently distributed. For this statistical model, the parameters are identifiable if $f(Re_i, Pr_i; \boldsymbol{\theta}) = \theta_1 Re_i^{\theta_2} Pr_i^{\theta_3} = \theta_1' Re_i^{\theta_2'} Pr_i^{\theta_3'} = f(Re_i, Pr_i; \boldsymbol{\theta}')$ implies that $\boldsymbol{\theta} = \boldsymbol{\theta}'$. We determine identifiability of the parameters using the Fisher information matrix $\mathcal{F}(\boldsymbol{\theta}) = \frac{1}{\sigma^2} \boldsymbol{S}^\top \boldsymbol{S}$ for the Dittus-Boelter equation, where

$$\boldsymbol{S} = \begin{bmatrix} \frac{\partial f}{\partial \theta_1}(Re_1, Pr_1; \boldsymbol{\theta}) & \frac{\partial f}{\partial \theta_2}(Re_1, Pr_1; \boldsymbol{\theta}) & \frac{\partial f}{\partial \theta_3}(Re_1, Pr_1; \boldsymbol{\theta}) \\ & \vdots & \\ \frac{\partial f}{\partial \theta_1}(Re_{56}, Pr_{56}; \boldsymbol{\theta}) & \frac{\partial f}{\partial \theta_2}(Re_{56}, Pr_{56}; \boldsymbol{\theta}) & \frac{\partial f}{\partial \theta_3}(Re_{56}, Pr_{56}; \boldsymbol{\theta}) \end{bmatrix}.$$

When the Fisher information matrix at the nominal values $\boldsymbol{\theta} = [0.023, 0.8.0.4]$ has full rank, then the parameters are locally identifiable around the nominal values. We can interpret the rank of the Fisher information at the nominal values by computing the singular values σ_i of $\boldsymbol{S}$

$$\Sigma = \begin{bmatrix} 5.01 \times 10^4 \\ 256 \\ 11.1 \end{bmatrix}.$$

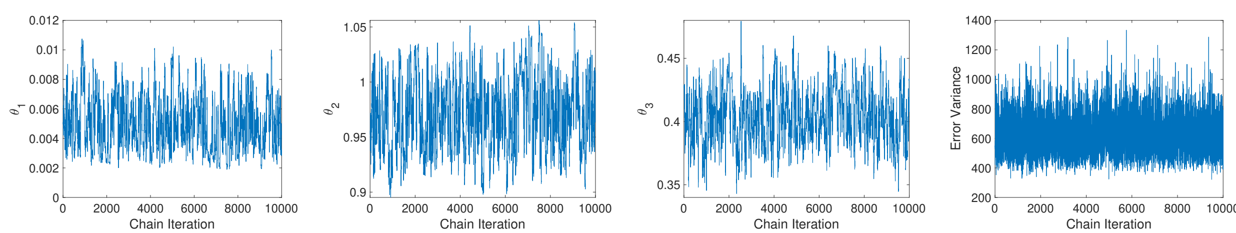
Since the singular values are non-zero, and $\sigma_i = \sqrt{\lambda_i}$, where λ_i are the eigenvalues of $\mathcal{F}(\boldsymbol{\theta})$, this shows that $\mathcal{F}(\boldsymbol{\theta})$ has full rank. We therefore conclude that the parameters are identifiable around the nominal values.

3 Bayesian inference

We now consider the Bayesian framework where $\boldsymbol{\theta}$ is treated as a random variable. With Bayesian inference, we would like to construct the distribution that $\boldsymbol{\theta}$ based on the likelihood of the fit to the observed data. We begin by choosing a prior distribution for $\boldsymbol{\theta}$. We pick a Gaussian prior while also imposing the constraint that $\theta_1 \geq 0$. This is informed by the physical constraint that the Nusselt number is positive. The nominal values $\boldsymbol{\theta} = [0.023, 0.8.0.4]$ are taken as the initial parameter values. We specify the initial error variance $\sigma^2 = 2.31 \times 10^4$ based on the variance with the nominal values

$$\sigma^2 = \frac{1}{56-3} \sum_{i=1}^{56} (0.023(Re_i)^{0.8}(Pr_i)^{0.4} - Nu_i)^2.$$

We construct the posterior distribution for $\boldsymbol{\theta}$ using the delayed rejection adaptive Metropolis (DRAM) algorithm [1], which provides updates for the covariance matrix with each chain iterate. Our DRAM implementation dedicates the first 10^4 iterations for burn in and constructs the posterior using an additional 10^4 iterations. The DRAM chains for $\boldsymbol{\theta}$ and for σ^2 are given in Fig. 1.

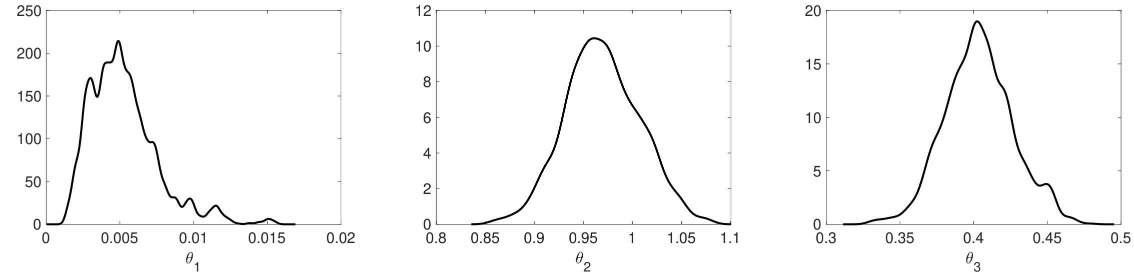


(a) (b) (c) (d)

Figure 1: DRAM chains for parameters $\boldsymbol{\theta}$, (a) (b) an (c), and error variance, (d), constructed for 10^4 iterations after 10^4 iterations of burn-in.

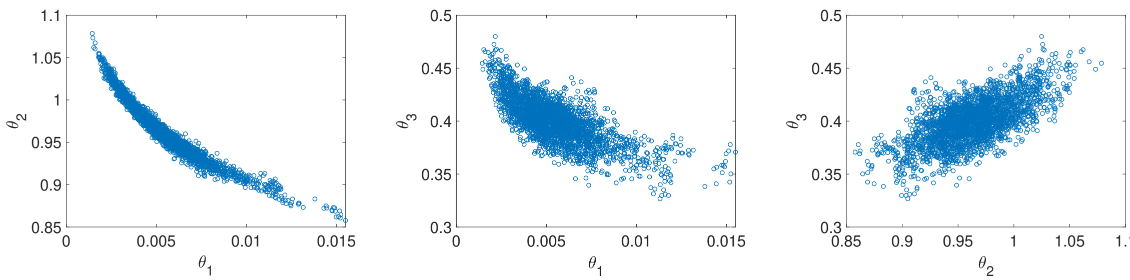
The means of the DRAM estimated posteriors are $\hat{\boldsymbol{\theta}} = [0.0054, 0.97, 0.40]$ with respective standard deviations $\mu_{\hat{\boldsymbol{\theta}}} = [0.0027, 0.041, 0.025]$. DRAM estimates the mean error variance as $\sigma^2 = 613.96$. We note that after burn-in, the parameter chains (a), (b), and (c) of Fig. 1 do not display ideal mixing behavior. We compare this to the chain for the error variance which does display the desired mixing behavior. The marginals of the posterior are given in Fig. 2.

We observe in (c) that the density of θ_3 is roughly symmetric while the other densities are not. Notably, the mean of θ_3 is the only estimated mean which corresponds closely to the respective



(a) (b) (c)

Figure 2: Marginal densities for parameters $\boldsymbol{\theta}$ constructed from DRAM chains.



(a) (b) (c)

Figure 3: Joint densities constructed from posterior distribution of $\boldsymbol{\theta}$

nominal value. The nominal value of θ_2, however, lies in a low density region of the posterior for θ_2, shown in (b) of Fig. 2. We now consider the pairwise plots for the parameters in Fig. 3.

We see that of the pairwise plots demonstrate patterns of correlations between the parameters. Particularly, we see a strong pattern of correlation between θ_1 and θ_2. We also note that the estimated means of these parameters diverge from their nominal values. These correlations explain why we do not observe ideal mixing behavior in Fig. 1. Nevertheless, we do still observe correlations are not so strong as to indicate the parameters are non-identifiable. Therefore, these results agree with the identifiability results. Based on how the parameter means diverge from the nominal values, this could issues with the assumed observation model (2), where the observation error term should be revised using experimental information.

References

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