STA 325 Case Study

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Introduction

Understanding fluid motion and turbulence is one of most challenging problems that physicists face. This case study will examine the relationship between three key properties of particles (Reynolds Number, Stokes Number, and Froude Number) and the probability distribution of particle cluster volumes. Through exploratory data analysis and nonlinear regression models, we are able to make predictions about the distribution of particle cluster volumes given parameter settings in terms of their four moments as well as better understand the way in which each parameter affects distribution.

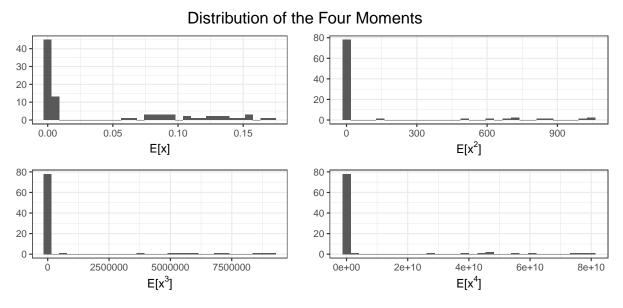
The dataset consists of 7 columns and 89 rows. Each row contains data from a simulation with different particle parameters. There are three predictor variables, or parameters:

Reynolds Number: a measure of the intensity of fluid turbulence of the particle. There are three values of Reynolds Number in the dataset: 90 (baseline value in regression), 224, and 338.

Stokes Number: a measure of the particle size and density. Values lie on the interval [0, 3] in the dataset.

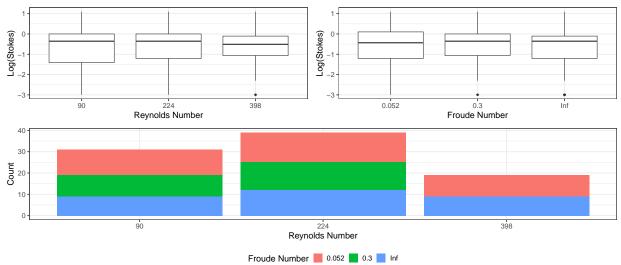
Froude Number: a measure of the gravitational acceleration of the particle. There are three values in the dataset: ∞ , 0.3, and 0.052 (baseline value in regression).

There are four response variables, which are each of the four moments ($\mathbb{E}[x]$, $\mathbb{E}[x^2]$, $\mathbb{E}[x^3]$, $\mathbb{E}[x^4]$) of the probability distribution function of Voronoï volumes. We can examine the distributions through histograms.



We can see that all four moments are right skewed and not normally distributed. We also wanted to examine the relationship between the predictors to determine if there is value in including interaction effects. To do so, we create boxplots to illustrate the relationship between the continuous and categorical variables (i.e. the relationship between Stokes Number and Reynolds/Froude Number).





We notice potential relationships between all three combinations of predictor variables, with particular emphasis on the differences in range of log Stokes values based on different Reynolds and Froude numbers. We also notice that there are no particles with a Froude number of 0.3 and a Reynolds number of 398.

Methodology

To examine the relationship between a particle's fluid turbulence, gravitational acceleration, and density on the four moments, we fit four nonlinear regression models with each moment as the response. We considered a number of transformations on each moment, such as a Box-Cox transformation, but ultimately decided to log transform each moment to have a clear interpretation of our subsequent regression coefficients. We also log transformed each particle's Stokes number as this predictor was far from normally distributed as well.

Regarding our predictors, we first converted both the Reynolds number and the Froude number of each particle to categorical predictors because there only existed three unique values for each parameter in the dataset and because the numerical differences between such values of Reynolds and Froude numbers were not easily interpretable. We posited from our background research that fitting three interaction, effects for all three predictors would better model the relationship between such predictors. For example, it is well established in existing research that fluid particle acceleration (Fr) is innately related to the turbulence of a flow (Re), in line with the Kolmogorov microscales. Therefore, we included all three potential interactions in our model (Stokes number interactions are log-transformed).

We also considered adding high order polynomials of the log of the Stokes number. We ran analysis of variance tests fitting models of varying degrees of log of the Stokes number and found that the quartic fit appeared to be reasonable for all moments. Therefore, our general model for each moment is as follows:

$$Y = \beta_0 + \beta_1 log(Stokes) + \beta_2 log(Stokes)^2 + \beta_3 log(Stokes)^3 + \beta_4 log(Stokes)^4 + \beta_5 Reynolds + \beta_6 Froude + \beta_7 (log(Stokes) * Froude) + \beta_8 (log(Stokes) * Reynolds) + \beta_9 (Froude * Reynolds)$$

Finally, we ran both stepwise forward and backward variable selections on each of our four models using AIC as our criteria. We personally care less about penalizing more complex models since we are given so few predictors to begin with anyways. Forward and backward selection did not remove or add any variables to the second, third, and fourth moment models, but did remove the interaction term between the Reynolds number and the log of the Stokes number for the first moment model. However, we still decided to include this interaction because we believe it is scientifically grounded.

Results

Here we display the results for our four regression models.

Table 1: Model 1

Table 3: Model 3

| | Estimate | Std. Error | $\Pr(> t)$ |
|----------------------|----------|------------|-------------|
| Intercept | -2.05 | 0.0199 | 7.05e-81 |
| Log(St) | 1.5 | 0.141 | 1.84e-16 |
| Log(St)^2 | 0.196 | 0.0698 | 0.0064 |
| Log(St)^3 | 0.471 | 0.0702 | 3.71e-09 |
| Log(St) ⁴ | -0.153 | 0.0706 | 0.0334 |
| Re 224 | -3.81 | 0.0288 | 9.75e-89 |
| Re 398 | -6.01 | 0.0311 | 1.22e-100 |
| Fr 0.3 | -0.237 | 0.031 | 5.94e-11 |
| Fr Inf | -0.272 | 0.0327 | 3.64e-12 |
| Fr 0.3 * Log(St) | 0.102 | 0.0184 | 4.7e-07 |
| Fr Inf * Log(St) | 0.0647 | 0.016 | 0.000123 |
| Re 224 * Log(St) | 0.0136 | 0.0155 | 0.382 |
| Re 398 * Log(St) | -0.0159 | 0.0203 | 0.436 |
| Re 224 * Fr 0.3 | 0.261 | 0.0401 | 8.57e-09 |
| Re 244 * Fr Inf | 0.381 | 0.0409 | 4.68e-14 |
| Re 398 * Fr Inf | 0.488 | 0.0446 | 4.81e-17 |

| | Estimate | Std. Error | $\Pr(> t)$ |
|----------------------|----------|------------|-------------|
| Intercept | 14.6 | 0.252 | 9.39e-63 |
| Log(St) | 19.3 | 1.79 | 1.07e-16 |
| Log(St)^2 | -8.55 | 0.886 | 1.14e-14 |
| Log(St)^3 | 6.72 | 0.891 | 1.01e-10 |
| Log(St) ⁴ | -3.61 | 0.895 | 0.000133 |
| Re 224 | -11.5 | 0.365 | 3.31e-44 |
| Re 398 | -18.1 | 0.395 | 1.76e-55 |
| Fr 0.3 | -13 | 0.393 | 8.41e-46 |
| Fr Inf | -13 | 0.415 | 4.19e-44 |
| Fr 0.3 * Log(St) | 0.14 | 0.234 | 0.55 |
| Fr Inf * Log(St) | -0.622 | 0.202 | 0.00298 |
| Re 224 * Log(St) | -0.312 | 0.196 | 0.116 |
| Re 398 * Log(St) | -1.08 | 0.257 | 7.65e-05 |
| Re 224 * Fr 0.3 | 8.97 | 0.508 | 4.9e-28 |
| Re 244 * Fr Inf | 8.74 | 0.519 | 7.14e-27 |
| Re 398 * Fr Inf | 13.2 | 0.566 | 1.21e-35 |

Table 2: Model 2

Table 4: Model 4

| | Estimate | Std. Error | $\Pr(> t)$ |
|----------------------|----------|------------|-------------|
| Intercept | 6.01 | 0.146 | 3.15e-52 |
| Log(St) | 12.1 | 1.04 | 2.4e-18 |
| Log(St)^2 | -5.01 | 0.514 | 7.86e-15 |
| Log(St)^3 | 4.12 | 0.517 | 1.58e-11 |
| Log(St) ⁴ | -2.16 | 0.52 | 8.74e-05 |
| Re 224 | -7.61 | 0.212 | 4.05e-48 |
| Re 398 | -12 | 0.229 | 1.28e-59 |
| Fr 0.3 | -6.74 | 0.228 | 2.24e-42 |
| Fr Inf | -6.76 | 0.241 | 7.56e-41 |
| Fr 0.3 * Log(St) | 0.108 | 0.136 | 0.428 |
| Fr Inf * Log(St) | -0.327 | 0.118 | 0.00694 |
| Re 224 * Log(St) | -0.136 | 0.114 | 0.236 |
| Re 398 * Log(St) | -0.627 | 0.149 | 7.48e-05 |
| Re 224 * Fr 0.3 | 4.75 | 0.295 | 1.01e-25 |
| Re 244 * Fr Inf | 4.68 | 0.301 | 7.22e-25 |
| Re 398 * Fr Inf | 6.99 | 0.329 | 5.15e-33 |
| | | | |

| | Estimate | Std. Error | $\Pr(> t)$ |
|----------------------|----------|------------|-------------|
| Intercept | 23.2 | 0.348 | 3.92e-67 |
| Log(St) | 25.6 | 2.48 | 6.41e-16 |
| Log(St)^2 | -11.6 | 1.22 | 2.03e-14 |
| Log(St)^3 | 9.01 | 1.23 | 2.59e-10 |
| Log(St) ⁴ | -4.87 | 1.24 | 0.000187 |
| Re 224 | -15.4 | 0.504 | 2.92e-43 |
| Re 398 | -24.1 | 0.545 | 1.97e-54 |
| Fr 0.3 | -19.2 | 0.543 | 8.88e-48 |
| Fr Inf | -19.2 | 0.573 | 4.96e-46 |
| Fr 0.3 * Log(St) | 0.153 | 0.323 | 0.637 |
| Fr Inf * Log(St) | -0.901 | 0.28 | 0.0019 |
| Re 224 * Log(St) | -0.468 | 0.271 | 0.0888 |
| Re 398 * Log(St) | -1.46 | 0.355 | 0.000103 |
| Re 224 * Fr 0.3 | 13.1 | 0.702 | 1.85e-29 |
| Re 244 * Fr Inf | 12.7 | 0.717 | 3.12e-28 |
| Re 398 * Fr Inf | 19.4 | 0.782 | 2.6e-37 |
| | | | |

The adjusted R-Squared values for each model were .9991, .9814, .9765, and .9757 respectively, indicating that essentially all of the variation in the log of the four moments can be explained by the combination of the predictor variables that we chose. Using an alpha of .05 as a threshold for statistical significance, we find that every individual predictor is statistically significant in each of the four models, though both the sign and magnitude of the coefficients vary by moment. We also notice that most of the interaction terms are also statistically significant, with the two clear exceptions being the interaction between a Froude number of 0.3 and log(Stokes) and the interaction between a Reynolds number of 224 and log(Stokes).

Let's first interpret the individual regression coefficients, starting with Stokes number. Recall that a higher Stokes number represents a larger and denser particle. We modeled a non-linear relationship between the log of the Stokes number and the moments, and so an interpretation of, say, a .1 unit increase in the Stokes number holding the Reynolds and Froude numbers constant, is not so clear. However, we do notice that for the second, third, and fourth moment model, the degree one and three coefficients are positive, while the degree two and four coefficients are negative.

Let's now examine the Froude number. Recall that high Froude numbers indicate that gravity can be neglected. The coefficients for the indicator variables of Froude are negative and essentially have the same magnitude for the two Froude values for all models, indicating that holding the size/density constant, a particle with a Reynolds number of 90 (baseline value) that experiences less influence from gravity (larger Froude values) is expected to have smaller moments than a particle that experiences influence from gravity.

Finally, we can examine the Reynolds number. Recall that high Reynolds numbers indicate that a particle's flow is turbulent and unpredictable. The coefficients for the standalone indicator values of Reynolds are negative, but the magnitude of the Reynolds indicator value of 398 is larger than then indicator value of 224. Holding the size/density constant, a particle with a Froude number of 0.052 (baseline value) that is more turbulent (larger Froude values) is expected to have smaller moments than a particle that is less turbulent.

Let's now examine the interaction between a particle's size and its gravitational influence (Froude number). We see that the interaction coefficient between log(Stokes) and a Froude number of 0.3 is positive for all four models, but that the coefficient between log(Stokes) and a Froude value of infinity is negative for the second, third, and fourth models. For particles that have such a high Froude value that they are in free fall, our model predicts that as they become larger and denser, holding turbulence constant, that their second, third, and fourth moments are expected to become smaller. This is in contrast to particles whose volume that experience more gravitational influence (Froude values of 0.3), in which as the particle becomes larger and denser, again holding turbulence constant, the second, third, and fourth moments of the distribution will become larger; however, this interaction was not statistically significant.

We can also examine the interaction between a particle's size and its turbulence (Reynolds number). We see that the interaction coefficient between log(Stokes) and a Reynolds number of 224 is only positive for the first moment model, but that the coefficient between log(Stokes) and a Reynolds value of 398 is negative for all the models (recall that the baseline value of Reynolds is 90). For particles that have such a high Reynolds value that they are extremely turbulent and unpredictable, our model predicts that as they become larger and denser, holding gravitational influence constant, that their second, third, and fourth moments are expected to become smaller. This effect is less pronouced for less turbulent particles (Reynolds number of 228); however, this interaction was not statistically significant.

Finally, we can examine the interaction effects between a particle's turbulence and gravitaional influence. We notice that all three interactions involving levels of the predictors are positive. Recall that the dataset did not contain any particles with a Froude number of 0.3 and a Reynolds number of 398, so we are missing one interaction term. We still notice that the magnitude of the interaction term with high turbulence (Reynolds value of 398) and no gravitational influence (Froude of infinity) is larger than the interaction term with medium turbulence (Reynolds value of 224) and no gravitational influence. This suggest that holding the size/density of the particle constant, particles with high turbulence and no gravitional influences are expected to have larger moments than particles with similar characteristics but less turbulence.