Neural Net Aided Solutions to Post Collision Behavior of Yield-Stress Fluids

Jack R. Goldrick

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Abstract

In the absence of governing equations, understanding the behavior of momentum in Yield-Stress Fluids (YSFs) can be rather difficult. These governing equations, such as a system of PDE's, are transformable to a non-unique non-dimensionalized space. A common method used is the Buckingham Pi Theorem which creates its famous pi-groups to accomplish the desired transformation. In 2015, TK Blackwell TK conducted an experiment to determine the post collision behavior of rheological fluids resulting in 5 regimes maps and a governing dimensionless variable that accurately describes the behavior. This study aims to develop a low resource neural net aided solution to identifying the behavior of the yield-stress fulids studied by Blackwell et al.

1 Introduction

1.1 Background

Yield-stress fluids are a vital resource in Industrial Engineering. These fluids are used in areas relating to agriculture and food processing, feedback control and safety systems, along with manufacturing [I Think I need to reference this]. Many of these processes can be aided by having real-time data driven methods that can provide an optimized and low-cost feedback control platform. Computational Fluid Dynamics (CFD) is extremely resource intensive and cannot be reliably used for real-time control. For reference, a simple T-Junction pipe flow solution from my undergrad took about 1.5hrs to fully render results on a GPU architecture. This glaring inefficiency overtly exceeds an acceptable time-to-compute (TTC) and must be optimized to handle scaling required by Industry. Many industry applications may involve fluid droplets contacting wet and/or dry surfaces and this simple difference can have dramatic consequences. To describe this difference, Blackwell [TK TK] denotes a situation where the parameter, surface hydrophobicity, may hold no predictive value, but the impact surface is completely wet prior to collision. This surface condition increases the minimum dimension of a model's parameter space. In the case described by Blackwell, the added parameter (dimension) is the thickness of the pre-coating layer which has high predictive value in models used to predict the collision behaviors of the described situation. So in the absence of governing equations how is one possibly supposed to arrive at the conclusion described by Blackwell?

1.2 Buckingham Pi

Since its discovery in the late 1800s as a generalization to the Rayleigh Method, the Buckingham Pi Theorem has become a quintessential tool used in dimensional analysis. The Buckingham Pi theorem states there exists a set of dimensionless quantities, known as π-groups, that span the full dimensionless solution space. A probabilistic corollary to the theorem states there must exist some function that projects a dataset to a lower dimensional space without a significant increase in the predictive error on the dataset [TK I think this needs a cite? it is heavily paraphrase from blackwell]. Blackwell's absence of governing equations makes Buckingham Pi the perfect analytical tool to gain a glimpse into the dynamics of momentum in Yield-Stress Fluids. It is important to note that may be fruitless to fully map all parameters, $p \in \mathbb{P}$, that dictate the full dynamics of a system. This fruitless overtone is a consequence of Buckingham Pi's one major pitfall: a set of π-groups derived from the solution is not unique. Properties such as shear viscosity have been shown to be quite difficult to measure and

can lead to a gap in necessary information for regression-based modeling, especially if the parameter has a high predictive value. Machine learning algorithms can circumvent the need to understand the governing dynamics thus making algorithms like SINDy unnecessary in applications described by Blackwell. This philosophy will be later used to derive a new use case for Buckingham Pi with respect to machine learning applications.

1.3 Machine Learning and Graphs

Given the general behavior of YSFs, there are many computational complexities and accuracy issues that arise from linear algorithms trying to predict high dimensional non-linear phenomena of YSFs. Certain machine learning algorithms have been shown to model well under these conditions and can provide the multi-class outputs needed to accurately model YSFs in the absence of a differential system. Ideally, these algorithms should help find some map $f : \mathbb{P} \to \mathbb{D}$ that maps every dimensional input parameter $\boldsymbol{p} \in \mathbb{P}$ to a classification category $\boldsymbol{d} \in \mathbb{D}$ such that error is minimized. Decision Tree and Neural Net based algorithms are readily equipped to fit and evaluate these kinds of datasets since they are both variations of Directed Acylic Computational Graphs (DACGs).

Definition 1.1 (Directed Acyclic Computational Graph) *A directed acyclic computational graph contains nodes, so that each node is associated with a variable. A set of directed edges connect nodes, which indicate functional relationships among nodes. Edges might be associated with learnable parameters. A variable in a node is either fixed externally (for input nodes with no incoming edges), or it is computed as a function of the variables in the tail ends of edges incoming into the node and the learnable parameters on the incoming edges.*

1.3.1 Decision Trees and Random Forests

Decision Trees are used to represent that ideal map f mentioned above. Generally, Decision Trees are comprised of nodes connected by unweighted directed edges. Decision Trees are analogous to a set of step-by-step instructions on computing the function value $f(\boldsymbol{p})$ given the features of each $\boldsymbol{p} \in \mathbb{P}$. Decision tree methods use as a hypothesis space the set of all hypotheses which represented by some collection of decision trees. A random forest expands on this by fitting a number of decision tree classifiers on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting. These methods search for a decision trees such that the corresponding hypothesis has minimum average loss on some labeled training data [TK Mostly quoted from keras documentation]. These models begin by feeding each $\boldsymbol{p}$ through a root node and outputting each $\boldsymbol{d}$ at a leaf node. A leaf node l, an edge-less node, represent a decision function $\mathcal{S}_l \subseteq \mathbb{P}$ in the feature space. The leaf nodes in the context of Blackwell's Data are the classification categories: the unique elements of $f(\mathbb{P})$.

1.3.2 Neural Networks and Deep Learning

2 Methodology

There was an issue with Bucki-Net that was ever present before the data was manipulated: What if Bucki-Net does not pick Blackwell's dimensionless variable as a π-group? Or worse: What if the data-driven output function is only surjective?

2.1 Data Manipulation and Buckingham Pi

2.2 Models

2.2.1 Decision Trees

2.2.2 Random Forests

2.2.3 Gradient Boosted Forests

2.3 Neural Networks

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$$S_n = \frac{X_1 + X_2 + \cdots + X_n}{n} = \frac{1}{n}\sum_{i}^{n} X_i$$

denote their mean. Then as n approaches infinity, the random variables $\sqrt{n}(S_n - \mu)$ converge in distribution to a normal $\mathcal{N}(0, \sigma^2)$.

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