Hierarchical Weibull Models for Predicting Batch-Level Ceramic Failure Strengths

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1 Problem Introduction

The strength of ceramic materials is determined by the distribution of flaws and their sizes within the material. The challenging processing conditions of ceramics and their sensitivity to impurities means that perfect ceramic fabrication is near impossible and will be variable across batches [1]. As such, it is common practice in industry to model the strength of ceramic materials by fitting them to a Weibull distribution, which is characterized by the probability density function given in Equation 1.

$$f(x) = \frac{\alpha}{\beta}\left(\frac{x}{\beta}\right)^{\alpha-1} \exp -(x/\beta)^k \tag{1}$$

Within the context of ceramics failure data, the parameters α and β take on specific meanings. The α parameter denotes characteristic strength of the material or the strength where 63.5% of ceramic specimens fail. The β parameter is referred to as the Weibull modulus and it describes the variability of the ceramic failure stress values, with a higher β value indicating a more consistent material.

Fitting the weibull distribution to ceramic failure data is typically performed through least squares or maximum likelihood estimation. However, such methods require a substantial amount of data ($n \geq 30$) for accurate fitting, which is both expensive and time consuming to collect [2]. For new materials, these rigorous testing requirements make sense and are wholly necessary. However, many companies are faced with need to characterize the same material on a batch to batch basis, with strength statistics showing strong similarity across batches. In such scenarios, it is likely that historical data could inform strength modeling so as to reduce sampling requirements. Furthermore, the application of probabilistic methods to parameter estimation can enable more rigorous uncertainty quantification of strength attributes.

This project aims to develop a Bayesian hierarchical model where shared α and β parameters can be learned across batches such that the strengths of subsequent ceramic batches can be characterized with lower data requirements.

2 Motivation

Materials science has historically been challenged by limited data, despite ever increasing pressure to produce new, novel materials. While there has been a lot of effort to introduce new machine learning techniques for materials discovery tasks, routine materials characterization tasks have received relatively little attention and many ceramicists continue to employ old techniques. The Bayesian approach offers a mathematical means of modeling and expressing uncertainty in low data scenarios, offering better predictions and better quantifying uncertainty in low data scenarios. Additionally the ability to specify historical and domain knowledge in the form of a prior provides an additional means of offsetting the limits of limited data [3].

This work aims to build a Bayesian hierarchical model for learning shared Weibull parameters across ceramic batches such that subsequent batches can be characterized through fewer experiments. Hierarchical models have traditionally, been used to model between and within group differences in studies of individuals and group structures [4]. A key advantage of the hierarchical approach is the ability to borrow predictive strength between groups such that groups with fewer samples can still benefit from the collective knowledge gained from the entire dataset [5]. This approach has two advantages over traditional approaches. First, the ability to share information across batches allows accurate predictions to be obtained with fewer samples. Second, the use of distributions to characterize the parameters of the weibull distribution provides a measure of uncertainty that can inform decision making.

3 Current Progress

To date, a simple, non-hierarchical Weibull model has been constructed to test the initial assumptions made in the motivation section and lay the groundwork for the next stages of the project. I have chosen to implement my model using the `PYMC` Python package which provides a tool set for Bayesian modeling using markov chain monte carlo (MCMC) estimation [citation]. Test my assumptions and validate the model, I have generated several synthetic datasets that are representative of batch-to-batch variability in ceramic materials. The specific parameter values for each dataset are shown in Table 1 and the distributions are plotted in Figure 1.

Table 1: Distribution parameters for the synthetic datasets.

Batch	**A**	**B**	**C**	**D**
Alpha	856.2	860.4	873.5	836.2
Beta	9.1	10.1	12.1	9.5

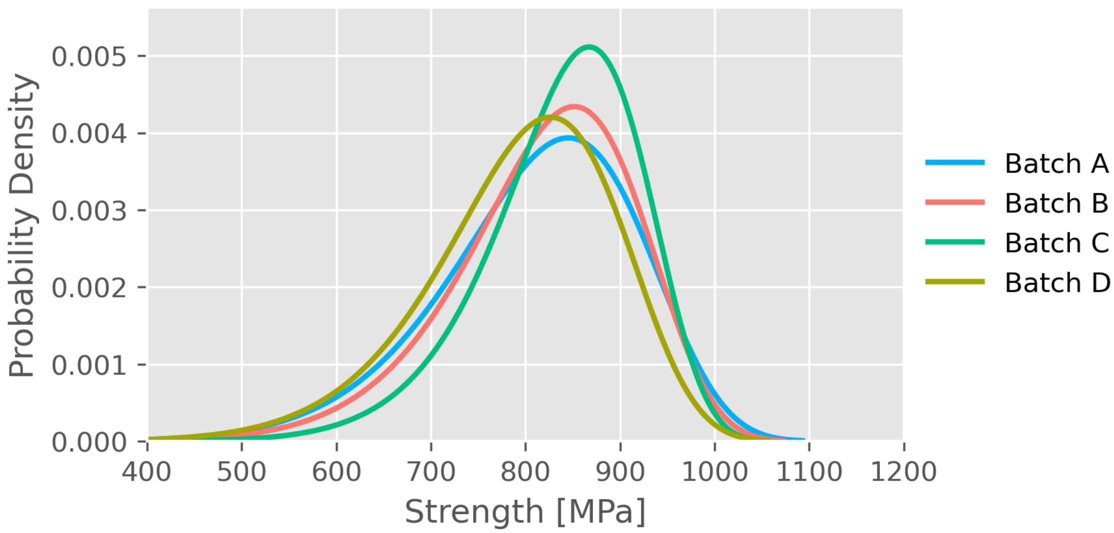

Figure 1: True distributions of synthetic datasets.

My assumption in implementing the hierarchical model is that having some prior or shared knowledge about the distribution of strength data can produce a more accurate estimate of Webiull parameters compared to an uninformed or frequentist estimation approach. To test this assumption I have constructed two variations of a Weibull fitting model using `PYMC` with uninformed and informed priors. The uninformed model has its parameters represented by uniform distributions spanning the plausible range of α and β values. The informed model has its parameters represented truncated normal distributions with the means near those specified for the synthetic data. A graphical representation of these models and their priors is shown in Figure 2. For frequentist estimate I am using the `reliability` package in python which includes tools for estimating weibull distribution parameters using maximum likelihood estimation.

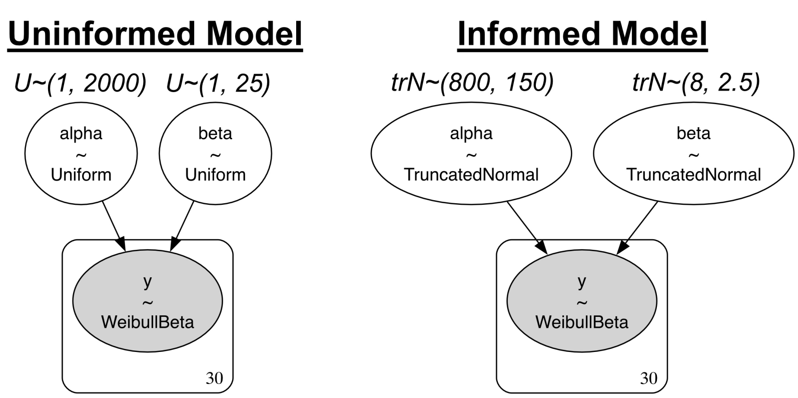

Figure 2: Diagrams of Bayesian Weibull models implemented in this work.

The fitting results are shown in Table 2. The batches are divided into four tables with the true values, MLE estimates, and MCMC estimates shown. For MLE, the estimated value and its standard error are reported, while the mean and standard deviation are reported for MCMC models. I observe that the frequentist and uninformed models perform similarly across each independent batch. These uninformed methods also tend to overestimate the beta parameter across all the synthetic datasets - showing overconfidence in the consistency of the sampled data. The informed model consistently shows closer estimates to the true beta value across all batches. However, it is noted that the uninformed and MLE methods show better characteristic strength estimation for Batch C and Batch D. This is likely an effect of the strength of the informed model's alpha prior. That said, the results show that there are benefits to informed priors for parameter estimating, which suggests a hierarchical approach could have some benefits in prediction.

Table 2: Fitting results for each model type across all batches.

Batch A				
	Alpha		Beta	
TRUE	856.2		9.1	
MLE	EST	SE	EST	SE
	862.9	16.3	10.1	1.5
MCMC	MU	STD	MU	STD
UNINFORMED	864.3	16.8	10	1.5
INFORMED	861.6	17.6	9.5	1.3

Batch B				
	Alpha		Beta	
TRUE	860.4		10.1	
MLE	EST	SE	EST	SE
	872.8	15.0	11.2	1.6
MCMC	MU	STD	MU	STD
UNINFORMED	874.1	15.6	11.1	1.6
INFORMED	871.1	16.4	10.3	1.3

Batch C				
	Alpha		Beta	
TRUE	873.5		12.1	
MLE	EST	SE	EST	SE
	871.4	11.7	14.4	2.1
MCMC	MU	STD	MU	STD
UNINFORMED	872.5	12.1	14.3	2.1
INFORMED	867.8	13.9	11.9	1.5

Batch D				
	Alpha		Beta	
TRUE	836.2		9.5	
MLE	EST	SE	EST	SE
	811.4	14.9	10.4	1.6
MCMC	MU	STD	MU	STD
UNINFORMED	813.0	15.6	10.4	1.6
INFORMED	810.8	15.8	9.7	1.3

4 Future Work

The work to date primarily aimed to test the assumption of an informative prior and lay the foundation for a later extension of the simple model to a hierarchical framework. This extension will be accompanied by a suite of tests wherein the model is trained on three of the batches and iteratively used to predict the the parameters the fourth batch as a function of observed data points. At each observation count iteration the basic MCMC and MLE models will also be tested to demonstrate the advantage of shared parameter information in the hierarchical model. Furthermore, several edge cases will be tested for synthetic batch datasets that show significant deviance from the those used in the hierarchical model to show the applicability of the model to outlier batches.

Following validation on synthetic data, the developed hierarchical model will be applied to a set of actual ceramics failure datasets to show performance on actual data, which is expected to be considerably more noisy and deviate from ideal behavior. This test will be essential to assessing the applicability of this method to real materials data and expose any shortcomings of the modeling approach.

5 Code Availability

The code associated with this project is available on github at the following public repository: `https://github.com/AndrewFalkowski/BayesianWeibullAnalysis`

References

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