Hierarchical Weibull Models for Predicting Batch-Level Ceramic Failure Strengths

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1 Problem Definition &Motivation

The strength of ceramic materials is determined by the distribution of flaws and their sizes within the material. The challenging processing conditions of ceramics combined with their sensitivity to impurities means that perfect ceramic fabrication is near impossible and will be variable across batches [1]. The failure of a ceramic material is known to be the result of the largest flaw within the material, which can be thought of as the weakest link in the material[2]. Thus, 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 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 [3]. 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 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.

2 Proposed Solution

A key assumption in batch-level analysis is that variability in batches stems from an unobserved distribution of processing parameters. In terms of the parameters α and β, it is expected that there are a set of global distributions from which a given batch's statistics are drawn. To model this, a hierarchcial Weibull model was developed that considers a set of batches that inherit their alpha and beta parameters from a global distribution of each. 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 [6]. A diagram of the model distributions and their priors is shown in Figure 1.

Priors on global parameters in the model were specified as uniform distributions bounded to realistic values for materials data. The choice of the uniform distribution was motivated by a desire to inject minimal bias into prior specification outside of establishing a realistic range for parameter values. Additionally, a computational motivation also guided uniform distribution bound selection as too large of bounds produced may divergences in the MCMC chains during computation.

The resulting global distributions are then fed into truncated normal distributions representing the α and β parameters for a weibull distribution over each batch. As material strength is strictly a positive number, the truncated normal allows a lower bound of zero to be set such that non-physical results are avoided. The set of global parameter distributions can then be thought of as priors on the α and β distribution parameters that come to reflect the mean distribution of each parameter. Put another way, the global parameter distributions characterize the most average batch's statistics - and thus can approximate batch-to-batch variability.

Analysis from midterm report suggested that informative priors could overcome the difficulties of estimating the parameters of weibull distributions. As informative priors are difficult to determine ahead of time, it is expected that a hierarchical model will automatically learn a set of informative priors in the global parameter distributions.

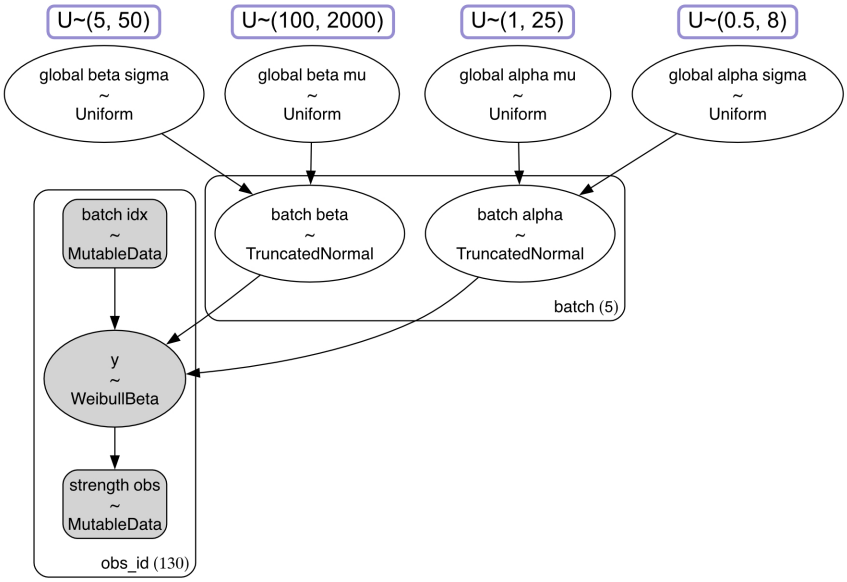

Figure 1: Diagram of Bayesian Hierarchical Model; priors on global parameters are circled above node icons.

3 Experimental Evaluation

To test the performance of the developed model, a set of synthetic datasets have been constructed. The use of synthetic datasets is motivated by the need to determine the accuracy of a model fit to a set of samples drawn from a given dataset. Obtaining true parameter estimates for real experimental dataset would require hundreds of samples to be collected, and even then, some error in estimation would be expected. Thus, by controlling the data generating process, I can more easily assess the accuracy of the model.

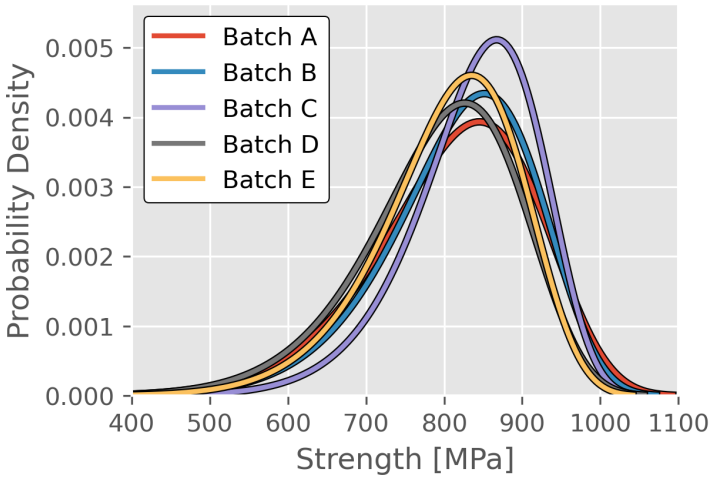

Figure 2: Synthetic dataset distributions.

Batch	Alpha	Beta
A	856.2	9.1
B	860.4	10.1
C	873.5	12.1
D	836.2	9.5
E	843.3	10.5

Table 1: Distribution parameters.

The parameter values used to construct each distribution in the synthetic dataset are shown in Table 3. The corresponding distributions are plotted in Figure 3. These parameter values were chosen based on reasonable estimates for batch-to-batch variability in silicon nitride ceramic test specimens. For batches A-D, 30 samples were drawn from each distribution to represent a set of observations. For Batch E, only 10 samples were drawn in order to assess how well the model estimates parameter values under limited sampling.

The model was fit using MCMC with the NUTS sampler with 15,000 burn-in and 10,000 samples over four chains. Fitting the model to Batches A-D, produces mixed results relative to a simple MLE fit. The fitting results are shown in Table 2, with the true parameters highlighted for clarity. In some cases, the MLE fit performs better, while in others the hierarchical model performs better. The difference stems from the implicit shrinkage phenomenon that is present in hierarchical models, which causes predicted values to skew towards the global mean values. This is seen in the case of Batch D, where the estimated value is pulled higher towards the global values in a beneficial way. By contrast, the estimated value for Batch C suffers as it is pulled down away from the true value. The advantage of the hierarchical approach is not immediately evident based on these results.

Table 2: Hierarchical vs. MLE fitting results.

			MLE		**Hierarchical**	
		TRUE	EST	SE	MU	STD
Batch A	Alpha	856.2	862.9	16.3	862.6	13.9
	Beta	9.1	10.1	1.5	10.5	1.3
Batch B	Alpha	860.4	872.8	15.0	869.1	13.9
	Beta	10.1	11.2	1.6	11.1	1.3
Batch C	Alpha	873.5	871.4	11.7	866.4	12.2
	Beta	12.1	14.4	2.1	12.6	1.7
Batch D	Alpha	836.2	811.4	14.9	825.9	15.9
	Beta	9.5	10.4	1.6	10.82	1.3
Global	Alpha				11.1	2.5
	Beta				855.9	27.9

Extending the hierarchical model to now predict Batch E with only 10 sampled points, provides several interesting results. First, despite a lower sample count, the model is able to estimate the parameter values of Batch E significantly better than the simpler MLE approach. This is attributed the shared information from prior higher sample count batches. Additionally, it is observed that the Batch E observations also change the hierarchical model estimates of the other batch parameters. In some cases these updated parameter estimates are better (Batch A, β: 10.5 $\rightarrow$ 10.3), but in others worse relative to the true values (Batch C, α: 866.4 $\rightarrow$ 864.8)). This suggests again the effect of shrinkage both in a positive and negative manner, but also the benefit of observing additional data groups in improving global parameter estimates.

Table 3: Hierarchical vs. MLE fitting results with Batch E.

			MLE		Hierarchical	
		TRUE	EST	SE	MU	STD
Batch A	Alpha	856.2	862.9	16.3	861.4	13.9
	Beta	9.1	10.1	1.5	10.3	1.3
Batch B	Alpha	860.4	872.8	15.0	867.2	13.9
	Beta	10.1	11.2	1.6	10.9	1.3
Batch C	Alpha	873.5	871.4	11.7	864.8	12.2
	Beta	12.1	14.4	2.1	12.3	1.7
Batch D	Alpha	836.2	811.4	14.9	825.5	15.9
	Beta	9.5	10.4	1.6	10.7	1.3
Batch E	Alpha	843.3	858.2	21.5	843.6	21.2
	Beta	10.5	13.3	3.5	10.0	1.7
Global	Alpha				10.8	2.1
	Beta				852.4	26.6

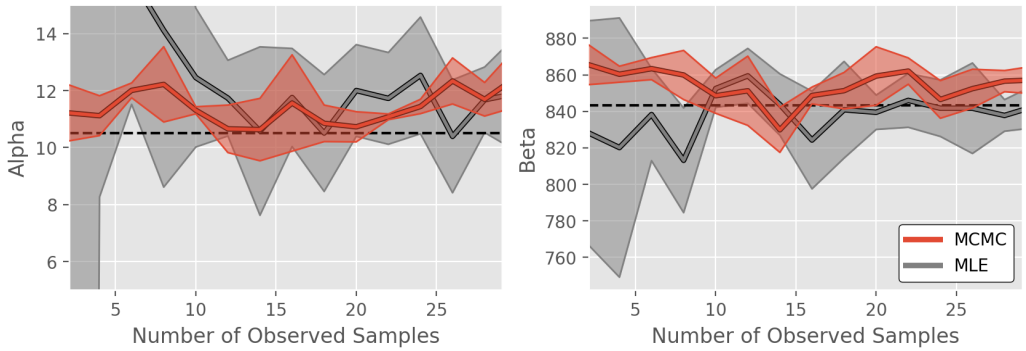

Figure 3: Convergence comparison between MLE and MCMC.

Finally, a convergence comparison is performed between the hierarchcial MCMC and MLE method for increasing numbers of Batch E observations. Figure 3 visualizes the estimated parameters for each model as a function of number of observed samples over five iterations. Both approaches feature a large amount of fitting noise. However, the hierarchical approach is consistently closer to the true parameters, even at low sample counts. This result suggests its value as a diagnostic tool under limited sampling conditions.

While the above results are promising, the Batch E results could in some sense be cherry picked to provide good results. The parameters of Batch E are within the range of the initial datasets, which is advantageous for hierarchical models. That said, batch-to-batch variability isn't expected to show high variability, in which case, such a model would be sufficient.

4 Future Work

The results presented in this work show the value of good prior specification in reducing sampling requirements in materials characterization. However, it is also clear that fitting approaches to the Weibull distribution need to be approached with caution as the inherent difficulty in observing and characterizing rare events leads to poor estimation. Both models have a tendency to over or underestimate the distribution values, even at $n = 30$ observations. To account for this, I plan to implement a corrective curve based on average fitting error that penalizes estimates based on the number of observations. At best this would provide more accurate estimates of ceramic strength, and at worst provide more conservative estimates of material properties. Additionally, information theory could be utilized to characterize the degree of convergence in parameter distributions. By examining the KL divergence between the prior and posterior at each iteration, estimated sampling requirements could be deduced on a case by case basis.

5 Code Availability

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

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