Bayesian Model Building From Small Samples of Disparate Data for 3D Printing

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Abstract
Quality control of geometric shape deformation in three-dimensional (3D) printing relies on statistical deformation models. However, resource constraints limit the

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manufacture of test shapes, and consequently impede the specification of deformation models for new shape varieties. We present a Bayesian methodology that effectively combines deformation data and models for a small sample of previously manufactured, disparate shapes to aid in the model specification of a broad class of new shapes. The power and simplicity of this general methodology is demonstrated with illustrative case studies on in-plane, or profile, deformation modeling for polygons and straight edges in free-form shapes using only data and models for cylinders and a single regular pentagon. Our Bayesian approach facilitates deformation modeling in general, and thereby can help advance 3D printing as a high-quality technology.

*Keywords:* Additive manufacturing, Bayesian data analysis, posterior predictive check, statistical shape analysis
The Challenge of Quality Control for 3D Printing Under Resource Constraints: Need for an Adaptive Methodology

Three-dimensional (3D) printing is a promising technology that enables the direct fabrication of complex shapes and eliminates the bulk and waste associated with traditional manufacturing (Campbell et al., 2011). A major issue that adversely affects its performance, and hence wider adoption, is that material solidification in the printing process yields geometric shape deformation (Wang et al., 1996). Several distinct “run-to-run” quality control methodologies have been developed, and are concisely summarized by Huang et al. (2014b, p. 061008–061009). For example, Tong et al. (2003, 2008) used observed deformation data to model a shape’s deformation separately in the $x$, $y$, and $z$ Cartesian coordinates. Such deformation models then inform the construction of a compensation plan, or modification of the shape’s computer-aided design model such that when the modified, new shape is printed, it deforms to more closely resemble the desired shape of interest. In contrast to such disjointed modeling approaches, Huang et al. (2015) conceived a new functional modeling strategy that effectively accounts for correlation in different coordinates and decouples geometric shape complexity from deformation modeling to construct compensation plans. The validation experiments of Huang et al. (2015, p. 439) have demonstrated that this approach can reduce deformation by one order of magnitude for the profiles of flat cylinders manufactured using stereolithography (Zhou and Chen, 2012).

A common feature of previously developed quality control methodologies for 3D printing is that they involve statistical deformation models for individual shapes, with no consideration paid to learning models for new shapes based on data and models for previous shapes.
Their associated common disadvantage is that physical experiments must be performed on several copies of each individual shape to specify their deformation models. Broad implementation of these methods is then made infeasible because the high operating cost of 3D printing limits the collection of deformation data to a small sample of distinct shapes. In fact, only a single, newly designed shape is typically printed in practice because of the huge variety of complex shapes that are of potential interest for future manufacture.

Thus a challenge in quality control of geometric shape deformation in 3D printing is the efficient specification of deformation models for new shapes using only the small sample of previously manufactured, different shapes. Huang et al. (2014b) attempted to address this challenge while building in-plane (2D) deformation models for circles, squares, pentagons and dodecagons. Their idea was to use the deformation model for circles proposed by Huang et al. (2015) as a key component in the deformation models for regular and irregular polygon shapes (under the assumption that a polygon deforms globally in a similar fashion as its circumcircle) and to add additional terms to capture the local deformation features. However, a major limitation of the approach was that, identification of the functions for capturing these local deformations was mostly heuristic in nature, and did not systematically utilize the existing data library on deformation. In addition, there did not exist a systematic approach for validation of the proposed models. These deficiencies apparently resulted in poor prediction from the postulated deformation models in certain cases.

Comment: Use a figure from our 2014b paper to show how the sawtooth function based model was unable to completely capture the pentagon deformation.

We address this challenge by developing a general adaptive Bayesian methodology for model building of a new shape’s in-plane, or profile, deformation based on one new sample
printed product and a small sample of products for a different shape in any 3D printing process. Our main contribution is to develop a framework for adaptively updating the deformation models built on the basis of data obtained from a limited number of tested shapes by successfully integrating data from one single new shape. The proposed approach utilizes the deformation model for circles used by Huang et al. (2015) and the “cookie cutter” conceptualization of deformation proposed by Huang et al. (2014b) (which links the deformation of a polygon to that of its circumcircle), but is essentially a novel approach for sequential or adaptive learning of deformation models in 3D printing.

The fundamental concepts that motivate our deformation modeling approach are contained in Sections 2.1 and 2.2. Section 2.3 describes the basic framework of our methodology, and how it can first facilitate learning about systematic deformation features unique to a new shape, and then enable the extension of the learned features to model deformation for new classes of shapes that are yet to be manufactured. The development of this framework into an adaptive learning methodology is described in Section 2.4. Our approach’s effectiveness is demonstrated via validation case studies in Section 3, which consider profile deformation modeling of polygons and the straight edges in free-form shapes using the deformation data and model for circles, with all shapes manufactured by stereolithography. These case studies are important, because previous applications of profile modeling in statistical shape analysis do not consider how the systematic components of past shapes’ models can be extended to new shapes in an efficient and simple manner. As we conclude in Section 4, our Bayesian methodology can not only help advance 3D printing as a high-quality technology, but can also contribute to shape analysis more broadly for both engineering and statistics.
2 Bayesian Model Building of Deformation Features

2.1 A Functional Representation of Shape Deformation

Throughout this article, we consider geometric shape deformation for profiles, or in-plane, two-dimensional shapes that correspond to individual layers of a 3D shape. We adopt the functional representation of deformation defined by Huang et al. (2015). This representation is obtained from transformation of the Cartesian \((x, y)\) coordinates of a manufactured shape into polar coordinates \((\theta, r)\), with \(\theta\) denoting the angle of a point (defined with respect to coordinate axes printed on the product) and \(r(\theta)\) its radius. Let \(r_{\gamma}^{\text{nom}}(\theta)\) and \(r_{\gamma}^{\text{obs}}(\theta)\) respectively denote the nominal and observed radius at angle \(\theta \in [0, 2\pi]\), where \(\gamma\) represents the known parameters (scalar or vector) that define the function \(r_{\gamma}^{\text{nom}}(\cdot)\). The parameter \(\gamma\) is scalar only for a circle, where it represents the radius, and typically a vector for other shapes. Huang et al. (2015, p. 432) define observed deformation at angle \(\theta\) as

\[
\Delta^{\text{obs}} r_{\gamma}(\theta) = r_{\gamma}^{\text{obs}}(\theta) - r_{\gamma}^{\text{nom}}(\theta).
\]

Figures 1(a) and 1(b) illustrate this definition for a circular product.

2.2 Modular Deformation Features for Different Shapes

We incorporate aspects of the “cookie-cutter” framework of Huang et al. (2014a,b) to explicitly connect deformation models of different shapes in a modular fashion via hypothesized additive deformation features. Consider two distinct shapes with nominal radius functions \(r_{\gamma_0}^{\text{nom}}, r_{\gamma_1}^{\text{nom}} : [0, 2\pi] \to \mathbb{R}\), respectively. In all that follows, \(r_{\gamma_0}^{\text{nom}}(\cdot)\) corresponds to a previously printed shape for which a deformation model has been learned from prior analyses, and \((\cdot)\) corresponds to one newly printed shape whose distinct deformation features remain to be
Figure 1: (a) The nominal shape versus the actual printed product. (b) The resulting deformation profile $\Delta r_{\text{nom}}^{\text{obs}}(\theta)$ plotted versus $\theta$ under the polar coordinate system.

discovered and modeled. Let the deformation model for $r_{\gamma_0}^{\text{nom}}$ be specified as

$$\Delta r_{\gamma_0}^{\text{obs}}(\theta) = \delta_{\gamma_0}(\theta|\alpha) + \epsilon_{\gamma_0}(\theta),$$

where the function $\delta_{\gamma_0}(\theta|\alpha)$ is a systematic deformation at $\theta$, $\alpha$ is a parameter vector assumed random in a Bayesian framework, and $\epsilon_{\gamma_0}(\theta)$ are random variables representing high-frequency deformation components with expectation $\mathbb{E}(\epsilon_{\gamma_0}(\theta)) = 0$ for all $\theta$ (Huang et al., 2015, p. 433–434). The systematic deformation feature of $r_{\gamma_0}^{\text{nom}}(\cdot)$ is then connected to the model of $r_{\gamma_1}^{\text{nom}}(\cdot)$ via a hypothesized additive cookie-cutter basis function, or local
deformation feature, $\delta_{\gamma_1}(\theta, \beta)$:

$$\Delta_{\text{obs}}^{\gamma_1}(\theta) = \delta_{\gamma_0}(\theta | \alpha) + \delta_{\gamma_1}(\theta | \beta) + \epsilon_{\gamma_1}(\theta)$$  \hspace{1cm} (3)

(Huang et al., 2014a,b). Function $\delta_{\gamma_0}$ captures a global deformation feature shared between $r_{\gamma_0}^{\text{nom}}(\cdot)$ and $r_{\gamma_1}^{\text{nom}}(\cdot)$, and $\delta_{\gamma_1}$ is a hypothesized, local deformation feature unique to the new shape, with parameter vector $\beta$. The $\epsilon_{\gamma_0}(\theta)$ and $\epsilon_{\gamma_1}(\theta)$ are assumed independent, with $\mathbb{E}(\epsilon_{\gamma_1}(\theta)) = 0$. Finally, note that both $\Delta_{\text{obs}}^{\gamma_1}(\theta)$ and $\Delta_{\text{obs}}^{\gamma_1}(\theta)$, in (2) and (3) respectively, satisfy (1).

The following illustrative example helps provide a physical justification for this modular deformation representation. Consider a regular polygon with $n$ edges and size (circumcircle radius) $r_0$, defined by the nominal radius function

$$r_{\gamma_1}^{\text{nom}}(\theta) = \frac{r_0 \cos\left(\frac{\pi}{n}\right)}{\cos\left\{\left(\theta - \frac{\pi}{2}\right) \mod \frac{2\pi}{n} - \frac{\pi}{n}\right\}},$$

where $\gamma_1 = (n, r_0)$, the two parameters that uniquely define the function. A polygon deformation model as hypothesized under this framework is then obtained by setting $r_{\gamma_0}^{\text{nom}}(\cdot) \equiv r_0$ (corresponding to the polygon’s size), where $\gamma_0 = r_0$, and using $r_{\gamma_1}^{\text{nom}}(\cdot)$ defined above in equation (3). To interpret this model specification, we recognize that, conceptually, the polygon deforms globally in a similar fashion as its circumcircle (Figure 2). We characterize $\delta_0$ as a global deformation feature shared between the polygon and its circumcircle. The regular polygon’s deformation systematically deviates from $\delta_0$ due to its straight edges and sharp corners, and $\delta_1$ is introduced to capture its corresponding local deformation features.

The task of deformation modeling for a new shape $r_{\gamma_1}^{\text{nom}}(\cdot)$ is thus reduced to specifying its local deformation feature $\delta_1$ based on one such newly printed product, because in practice the specification of its global deformation feature is known from previous stud-
Figure 2: The pentagon deforms globally in a similar manner as the expected deformation of its circumcircle, and systematic deviations are introduced locally due to its edges.

Huang et al. (2014b, p. 0610086–0610087) considered the application of pre-specified square wave and sawtooth functions for the local deformation feature of polygonal shapes. However, modeling local deformation features based on pre-specified functional forms may not yield success in practice because it is typically extremely difficult to conceive \textit{a priori} of parsimonious and appropriate local deformation feature specifications for complex shapes. An alternative approach that is more justifiable from a statistical perspective is to directly learn local deformation features that persist across shapes based on a combination of prior inferences for $\delta_0$ and observed deformation data $r_{\gamma_1}^{\text{obs}}(\theta)$ for a newly printed shape $r_{\gamma_1}^{\text{nom}}(\cdot)$. Our methodology is directly geared to accomplish this learning task, and is described next.
2.3 A New Approach for Modeling the Local Deformation Feature $\delta_1$

Our Bayesian model building methodology proceeds in three steps. First is the construction of a discrepancy measure (Rubin, 1984; Meng, 1994) to extract information on the local deformation feature $\delta_1$ for a new shape $r_{\gamma_1}^{\text{nom}}(\cdot)$, using the data for only a single newly manufactured shape and posterior inferences for the parameters $\alpha$ of its global deformation feature based on previously manufactured shapes $r_{\gamma_0}^{\text{nom}}(\cdot)$. Second is blocking the discrepancy measure distributions according to covariates thought to explain the local deformation feature, and comparing the distributions within and across blocks to identify and test for systematic trends in the local deformation feature as a function of $\theta$ and $r_{\gamma_1}^{\text{nom}}(\cdot)$. Third is to specify a hierarchical model across the blocks for the parameters $\beta$ of the previously identified trends such that the local deformation feature model specification for $r_{\gamma_1}^{\text{nom}}(\cdot)$ can be directly extended to a broad class of shapes that share similar features as $r_{\gamma_1}^{\text{nom}}(\cdot)$.

The first step in our procedure is accomplished through consideration of equation (3). Let $D_{\gamma_0}$ denote deformation data $r_{\gamma_0}^{\text{obs}}(\theta)$ for manufactured shapes with nominal radius function $r_{\gamma_0}^{\text{nom}}(\cdot)$, and $F(\alpha \mid D_{\gamma_0})$ the posterior distribution of $\alpha$ based on $D_{\gamma_0}$. Our discrepancy measure is defined by the transformation of the observed deformation data $\Delta^{\text{obs}} r_{\gamma_1}(\theta)$ for a single, newly manufactured shape into the random variable

$$T_{\gamma_1}(\theta) = \Delta^{\text{obs}} r_{\gamma_1}(\theta) - \delta_{\gamma_0}(\theta|\tilde{\alpha}),$$  

(4)

where $\tilde{\alpha} \sim F(\alpha \mid D_{\gamma_0})$. This transformation effectively removes the potentially non-trivial global deformation feature inherent in the new shape from its deformation data, so as to permit one to focus on the local deformation feature. Alternatively, this discrepancy measure provides a simple and concrete starting point to learn a functional form of $\delta_1$ in
terms of $\theta$ and $\gamma_{11}^{\text{nom}}(\theta)$ using inferences from the small set of previously manufactured and different shapes. The distribution of this discrepancy measure is most conveniently derived via Monte Carlo: if $\tilde{\alpha}(l) \sim F(\alpha \mid D_{\gamma_{10}})$ for $l = 1, \ldots, L$, then $L$ draws from the distribution of the discrepancy measure in equation (4) are obtained as

$$T_{\gamma_{11}}^{(l)}(\theta) = \Delta_{\text{obs}} \gamma_{11}^{\text{obs}}(\theta) - \delta_{0}(\theta|\tilde{\alpha}(l)).$$  

(5)

After the distributions of the discrepancy measure defined in equation (4) are obtained, we proceed in our second step to group them into $E$ blocks defined a priori by covariates thought to be associated with the local deformation feature (e.g. for a polygon shape, each side can be taken as a block), and test for and specify systematic trends in $T_{\gamma_{11}}(\theta)$ as a function of $\theta$ and $\gamma_{11}^{\text{nom}}(\theta)$, within and across blocks. Traditional testing methods generally involve the construction of real-valued functions of data to detect specific trends of interest. However, such methods may not be particularly useful in this context for the same reason why pre-specified local deformation features may not yield success in deformation modeling, specifically, the complexity of local deformation features in new shapes. We accordingly construct two types of graphical posterior predictive checks (Gelman et al., 1996; Gelman, 2003) that enable identification and testing of local deformation feature trends in a flexible manner. The first consists of plots of distributional summaries of the discrepancy measures (e.g., the mean and 0.025, 0.975 quantiles) against the nominal radius function $\gamma_{11}^{\text{nom}}(\theta)$, stratified according to the $E$ blocks. We use the uncertainty measures summarized in these plots to test for visually identifiable trends in local deformation as a function of $\theta$, $\gamma_{11}^{\text{nom}}(\theta)$ within each block $e = 1, \ldots, E$. For example, we can use the central 95% intervals of $T_{\gamma_{11}}(\theta)$ to test groups of points $\theta$ within each block $e$ that exhibit a particular trend of $T_{1}(\theta)$ as a function of $(\theta)$. An example of such a trend is $T_{\gamma_{11}}(\theta)$ being a parabolic function of $\gamma_{11}^{\text{nom}}(\theta)$.
within each block, as will be seen later in an example in Section 3.

After testing using this first graphical posterior predictive check and obtaining the $K$ distinct trends of $T_{\gamma_1}(\theta)$ as a function of $\theta$ and $r_{\gamma_1}^{\text{nom}}(\theta)$ that exist across the blocks $e = 1, \ldots, E$, we group all points $\theta$ into clusters $\Theta_k$, $k = 1, \ldots, K$, that constitute the previously identified local deformation feature trends.

The second graphical posterior predictive check consists of plots of distributional summaries of the discrepancy measure against $r_{\gamma_1}^{\text{nom}}(\theta)$, stratified according to these $K$ clusters. We now use the uncertainty measures contained in these plots to verify, for each cluster $\Theta_k$, the identical nature of the associated systematic trend of $T_{\gamma_1}(\theta)$ as a function of $\theta$ and $r_{\gamma_1}^{\text{nom}}(\theta)$ over all blocks $e = 1, \ldots, E$. The second step of our procedure concludes by using the results and observations from these two graphical posterior predictive checks to model the local deformation feature for $r_{\gamma_1}^{\text{nom}}(\cdot)$ as

$$
\delta_{\gamma_1}(\theta|\beta) = \sum_{k=1}^{K} \mathbb{1}(\theta \in \Theta_k) \delta_{\gamma_1,k} \left( \theta | \beta_{e(\theta),k} \right),
$$

where $e : [0, 2\pi] \to \{1, \ldots, E\}$ is the indicator function for the block level of $\theta$, and $\delta_{\gamma_1,k}$ corresponds to the $k$th distinct trend of the local deformation feature. The functional form of $\delta_{\gamma_1,k}$ is constant across blocks $e = 1, \ldots, E$, but the parameters $\beta_{e,k}$ are distinct across block levels $e$ and trends, with the $\beta_{e,k}$ concatenated into $\beta$.

The third step of our procedure is to specify hierarchical models on the $\beta_{e,k}$ across blocks, i.e., for $k = 1, \ldots, K$,

$$
\beta_{1,k}, \ldots, \beta_{E,k} | \psi_k \sim p(\psi_k),
$$

and place non-informative priors on the hyperparameters $\psi_1, \ldots, \psi_K$. Such a hierarchical
model will allow us to make full use of the previously identified local deformation feature trends across blocks. For example, this model structure enables us to pool the observed deformation data for points \( \theta \) on a newly manufactured shape \( r_{\gamma_1}^{\text{nom}}(\cdot) \) that reside in the same cluster \( \Theta_k \), and thereby improve the inferential precision for the model parameters. This improvement is especially important in light of the complication of small samples of new shapes that can be manufactured. Furthermore, this hierarchical structure is sufficiently general so as to enable the immediate extension of the learned local deformation feature model from one shape \( r_{\gamma_1}^{\text{nom}}(\cdot) \) to new shapes that share similar features with \( r_{\gamma_1}^{\text{nom}}(\cdot) \).

It is important to note that, after specifying the complete model for \( \delta_{\gamma_1} \) in the third step, we proceed to fit the full deformation model involving both \( \delta_{\gamma_0} \) and \( \delta_{\gamma_1} \) to the observed data \( r_{\gamma_0}^{\text{obs}}(\cdot) \) and \( r_{\gamma_1}^{\text{obs}}(\cdot) \). Specifically, shapes with nominal radius function \( r_{\gamma_0}^{\text{nom}}(\cdot) \) will have their \( \delta_{\gamma_1}(\cdot) \equiv 0 \), and \( \delta_{\gamma_0}(\cdot) \) is shared between the two types of shapes. This further enables the full use of all data for efficient inferences in this constrained context.

2.4 An adaptive Bayesian learning procedure

In the previous subsection we presented a basic framework for learning about the deformation about a new shape \( r_{\gamma_1}^{\text{nom}}(\cdot) \) combining observed data \((\theta, r_{\gamma_0}^{\text{obs}}(\theta))\) on a previously manufactured shape \( r_{\gamma_0}^{\text{nom}}(\cdot) \) and new data \((\theta, r_{\gamma_1}^{\text{obs}}(\cdot))\) from the new shape. This framework can easily be generalized to an adaptive learning procedure as described next. Assume that our data bank now has data \( D_{\text{current}} \) on a library of \( J \) current shapes whose nominal radius functions are parametrized by \( \gamma_1, \ldots, \gamma_J \). The deformation models for these \( J \) shapes involve a set of functions \( \delta_{\text{current}} = \{\delta_{\gamma_1}(\theta|\beta_1), \ldots, \delta_{\gamma_J}(\theta|\beta_J)\} \) and a collection of parameters \( \beta_{\text{current}} = (\beta_1, \ldots, \beta_J) \).

Now suppose we observed data \( D_{J+1} \) from a single replicate of a new shape with nominal radius function parametrized by \( \gamma_{J+1} \). Assuming that the deformation of the \((J + 1)\)th
shape shares common features with the current library of shapes, we learn about the unique features of its deformation through the function $\delta_{\gamma,J+1}(\theta|\beta_{J+1})$ using the discrepancy measure $T_{\gamma,J+1}(\theta)$. This discrepancy measure is a function of the observed deformation $\Delta_{\text{obs}}^{\gamma,J+1}(\theta)$ of the $(J+1)$th shape, and the set of known functions $\delta_{\text{current}}$. The distribution of this test statistic is generated as in (5) using posterior draws of $\beta_{\text{current}}$ given $D_{\text{current}}$.

The graphical posterior predictive checks described in the previous subsection then helps us postulate a model for $\delta_{\gamma,J+1}(\theta|\beta_{J+1})$. We put priors on $\beta_{J+1}$, update the current data to $(D_1, \ldots, D_{J+1})$, the class of functions to $\{\delta_{\gamma_1}(\theta|\beta_1), \ldots, \delta_{\gamma,J+1}(\theta|\beta_{J+1})\}$ and the ensemble of parameters to $(\beta_1, \ldots, \beta_{J+1})$, and obtain posterior distributions of the vector of parameters $(\beta_1, \ldots, \beta_{J+1})$ given the augmented data set. Therefore the posterior distributions of the parameters are updated after each step of this adaptive learning process.

3 Deformation Model Building for Polygons and the Straight Edges in Free-Form Shapes

3.1 Learning From Cylinders and a Single Regular Pentagon

We present case studies of our Bayesian methodology for deformation modeling of polygons and the straight edges in free-form shapes based on one manufactured regular pentagon and three manufactured flat cylinders. Section 3.2 summarizes a Bayesian analysis of cylinder deformation based on the work of Sabbaghi et al. (2015). Our procedure is then applied, using the posterior distribution of the global deformation feature model parameters derived from cylinders, and the observed deformation for a single regular pentagon, to build a general local deformation feature model for polygons and the straight edges in free-form shapes in Section 3.3. The blocks in this case are intervals of angles corresponding to
each individual straight edge in a shape, and the clusters identified in the second step of
our procedure are defined with respect to angles $\theta$ that have the minimum nominal radius
for each level of the blocking factor. We illustrate a validation of this model for shapes
with a similar local deformation feature as the regular pentagon by considering the model
fit for a newly manufactured irregular polygon in Section 3.4. Our second validation is
performed for a poorly compensated pentagon in Section 3.5, and this study illustrates
that the learned local deformation feature persists for the straight edges of a shape whose
boundary involves free-form segments.

3.2 Flat Cylinders and the Global Deformation Feature Model

Sabbaghi et al. (2015, p. 908) analyzed the shape deformations of approximately 1000
equally-spaced points for each of three flat cylinders of nominal radii $\gamma_0 = 0.5''$, $1.5''$, and
3'' (Figure 3) manufactured by stereolithography. The magnitude of the deformations
increases in $\gamma_0$. The $\gamma_0 = 1.5''$ and $3''$ cylinders have positive deformation (i.e., are larger
than desired) because the 3D printer overcompensated under its settings (Huang et al.,
2014b, p. 061011). Distinct deformation profiles exist in their top and bottom halves.

We adopt as the global deformation feature model the cylinder deformation model of
Sabbaghi et al. (2015, p. 908), which is a special form of (2), and is

$$
\Delta_{\text{obs}} r_{\gamma_0}(\theta) = \delta_{\gamma_0}(\theta|\alpha) + \epsilon_{\gamma_0}(\theta)
$$

$$
= \mathbb{I}(0 \leq \theta \leq \pi)\delta_{\gamma_0,U}(\theta|\alpha) + \{1 - \mathbb{I}(0 \leq \theta \leq \pi)\} \delta_{\gamma_0,L}(\theta|\alpha) + \epsilon_{\gamma_0}(\theta),
$$

with

$$
\mathbb{I}(0 \leq \theta \leq \pi) = \begin{cases} 
1 & \text{if } 0 \leq \theta \leq \pi, \\
0 & \text{otherwise}, 
\end{cases}
$$
Deformation and Model Fit for Three Manufactured Cylinders

Figure 3: Observed deformations (gray dots), and posterior predictive means (solid lines) and 95% central posterior predictive intervals (dashed lines), for three flat cylinders of nominal radii $\gamma_0 = 0.5''$, $1.5''$, and $3''$. The dashed vertical line demarcates the upper and lower halves.

$$
\delta_{\gamma_0,U}(\theta|\alpha) = x_{0,U} + \alpha_{0,U}(\gamma_0 + x_{0,U})^{a_{0,U}} + \alpha_{1,U}(\gamma_0 + x_{0,U})^{a_{1,U}} \cos\{2(\theta - \psi_U)\},
$$

$$
\delta_{\gamma_0,L}(\theta|\alpha) = x_{0,L} + \alpha_{0,L}(\gamma_0 + x_{0,L})^{a_{0,L}} + \alpha_{1,L}(\gamma_0 + x_{0,L})^{a_{1,L}} \cos\{2(\theta - \psi_L)\},
$$

and $\epsilon_{\gamma_0}(\theta) \sim \text{iid} N(0, \sigma_0^2)$. Similar to the analyses of Sabbaghi et al. (2014, p. 1401, 1411–1413), independent residuals are considered because our primary objective is to learn the systematic local deformation features for new shapes based on inferences for the global deformation feature. Vector $\alpha$ contains the 12 parameters above, excluding $\sigma_0^2$. Parameters $x_{0,U}$ and $x_{0,L}$ account for over-/under-exposure in stereolithography, defined as either the expansion (over-exposure) or contraction (under-exposure) of an illuminated shape due to the spread of light beams on its boundary (Sabbaghi et al., 2015, p. 908). Huang et al.
(2015, p. 438–440) previously considered over-exposure, i.e., positive $x_{0,U}$ and $x_{0,L}$, as their $\gamma_0 = 0.5''$ cylinder expanded to yield positive deformation. Figure 3 suggests under-exposure, i.e., negative $x_{0,U}$ and $x_{0,L}$, because the $\gamma_0 = 0.5''$ cylinder contracts to yield negative deformation for $\theta \in [0, 3\pi/2)$.

Sabbaghi et al. (2015, p. 908) adopted a specific prior distribution for $\alpha$, and assumed all model parameters were independent \textit{a priori}. Although we also assume prior independence of the global deformation feature model parameters, we specify a different prior on $\alpha$, which is further described in the appendix. After specifying our prior, we then fit this model to the cylinder deformation data via Hamiltonian Monte Carlo (Duane et al., 1987), with 1000 posterior draws of $\alpha$ and $\sigma^2_0$ obtained after a burn-in of 500. The posterior mean, and 0.025 and 0.975 posterior quantiles, of deformation for each $\theta$ are plotted in Figure 3. Similar to the work of Sabbaghi et al. (2015, p. 908), this figure demonstrates that the specified $\delta_0$ performs well in capturing cylinder deformation. We proceed to use this $\delta_0$ as the global deformation feature for new polygons.

3.3 Learning a Local Deformation Feature Model From a Single Polygon

We now apply our Bayesian model building methodology to specify a local deformation feature model for a broad class of new shapes based on our previous inferences for the cylinder global deformation feature and the observed deformation for a different shape. Specifically, we consider a new regular pentagon of size $3''$ and nominal radius function

$$r_{\gamma_1}^{\text{nom}}(\theta) = \frac{3\cos\left(\frac{\pi}{5}\right)}{\cos\left\{\left(\theta - \frac{\pi}{2}\right) \mod \frac{2\pi}{5} - \frac{\pi}{5}\right\}}.$$
Figure 4: Observed deformation (gray dots) for a new 3″ regular pentagon.

with $\gamma_1 = (5, 3)$, whose deformation is displayed in Figure 4. The broad class of shapes in this case includes regular and irregular polygons, and the straight edges in free-form shapes.

The first step of our procedure follows by taking $r_{\gamma_0}^{\text{nom}}(\theta) \equiv 3$ and using the inferences performed in Section 3.2. For every point $\theta$ on the new pentagon, we form a Monte Carlo approximation of $\delta_{\gamma_0}(\theta|\tilde{\alpha})$ using posterior draws of $\alpha$ based on the cylinder data, and then construct the Monte Carlo approximation of the distribution of $T_{\gamma_1}(\theta)$.

We next construct the two graphical posterior predictive checks to identify and test for local deformation feature trends. In this case, the edges of the polygon (labeled in Figure 5) constitute natural blocks, because of the symmetry in $r_{\gamma_1}^{\text{nom}}(\cdot)$ across its edges. Accordingly, summaries of the distributions of the discrepancy measure are stratified according to these blocks in Figure 6. We immediately identify two consistent trends within each block: for
nearly half the points \( \theta \), the expectation of their discrepancy measure increases as a function of \( r_{\gamma_1}^{\text{nom}}(\theta) \), and for the remaining points, the expectation decreases as a function of \( r_{\gamma_1}^{\text{nom}}(\theta) \). Furthermore, a transition point for the trend within a block occurs at \( r_{\gamma_1}^{\text{nom}}(\theta) = 3\cos(\pi/5) \), which is the minimum value of \( r_{\gamma_1}^{\text{nom}}(\theta) \) within the block. A test of these trends based on the central 95% intervals of the discrepancy measure distributions within each block verifies that they are distinct. The local deformation feature is more complicated near the sharp corners, and these trends do not hold for all of the small number of points \( \theta \) with \( r_{\gamma_1}^{\text{nom}}(\theta) > 2.98 \), which we exclude from consideration. We use the results of the first graphical posterior predictive check to group all points into two distinct clusters \( \Theta_1 \) and \( \Theta_2 \), corresponding to the half-edges that have a positive trend in the discrepancy measure and those that have a negative trend, respectively, as a function of \( r_1(\theta) \). The second graphical posterior predictive check that stratifies the distributional summaries of the discrepancy measure across these two clusters is in Figure 7. We conclude from inspection of the uncertainty measures and correspondence of trends in these plots that the identified trends are identical across blocks. These tests yield the local deformation feature model

\[
\delta_{\gamma_1}(\theta|\beta) = \sum_{k=1}^{2} \mathbb{I}(\theta \in \Theta_k) \delta_{\gamma_1,k}(\theta|\beta_{\epsilon(\theta),k}),
\]

where

\[
\delta_{\gamma_1,k}(\theta|\beta_{\epsilon(\theta),k}) = \beta_{\epsilon(\theta),0} + \beta_{\epsilon(\theta),1,k} \left\{ r_{\gamma_1}^{\text{nom}}(\theta) - r_{\gamma_1}^{\text{nom}}(m(\theta)) \right\}^{b_k(\theta),k},
\]

with \( m : [0, 2\pi] \rightarrow [0, 2\pi] \) defined as

\[
m(\theta) = \arg\min_{t : \epsilon(t) = \epsilon(\theta)} r_{\gamma_1}^{\text{nom}}(t),
\]

and \( \epsilon : [0, 2\pi] \rightarrow \{1, 2, 3, 4, 5\} \) is the function that returns the block containing \( \theta \) (Figure 5).
Five new parameters are introduced for each block, with $\beta_{e(\theta),1,1}$, $b_{e(\theta),1}$ and $\beta_{e(\theta),2,1}$, $b_{e(\theta),2}$ corresponding to the two identified, distinct systematic trends that exist across blocks.

The different magnitudes for each trend across blocks is accommodated through the specification of hierarchical models on $\beta_{e(\theta),0}$, $\beta_{e(\theta),1,1}$, and $\beta_{e(\theta),2,1}$, and weakly informative priors on $b_{e(\theta),1}$ and $b_{e(\theta),2}$ in the final step of our procedure. Specifically, we let

$$\beta_{1,0}, \beta_{2,0}, \beta_{3,0}, \beta_{4,0}, \beta_{5,0} \overset{iid}{\sim} N(\mu_0, \tau_0^2),$$

$$\beta_{1,1,1}, \beta_{2,1,1}, \beta_{3,1,1}, \beta_{4,1,1}, \beta_{5,1,1} \overset{iid}{\sim} N(\mu_1, \tau_1^2),$$

$$\beta_{1,2,1}, \beta_{2,2,1}, \beta_{3,2,1}, \beta_{4,2,1}, \beta_{5,2,1} \overset{iid}{\sim} N(\mu_2, \tau_2^2),$$

$$b_{1,1}, b_{2,1}, \ldots, b_{5,1}, b_{1,2}, b_{2,2}, \ldots, b_{5,2} \overset{iid}{\sim} N\left(\frac{1}{2}, 1^2\right),$$
Figure 6: Plots of the mean and 0.025 and 0.975 quantiles of the $3''$ regular pentagon’s discrepancy measure as a function of $r_1^\text{nom}(\theta)$ for each block, with a vertical dashed line at 2.98.
with all parameters mutually independent \( a \ priori \). The standard reference prior

\[
p \left( \mu_0, \mu_1, \mu_2, \tau_0^2, \tau_1^2, \tau_2^2 \right) \propto \frac{1}{\tau_0 \tau_1 \tau_2}
\]

is placed on the hyperparameters.

We fit the following model, including priors on \( \alpha, \beta \), and \( \sigma_0^2 \), to all the previous shapes:

\[
\Delta_{\text{obs}} r_{\gamma_0}(\theta) = \delta_{\gamma_0}(\theta|\alpha) + \epsilon_{\gamma_0}(\theta),
\]

\[
\Delta_{\text{obs}} r_{\gamma_1}(\theta) = \delta_{\gamma_0}(\theta|\alpha) + \delta_{\gamma_1}(\theta|\beta) + \epsilon_{\gamma_1}(\theta).
\]

Residuals \( \epsilon_{\gamma_0}(\theta) \) \( \text{iid} \sim N(0, \sigma_0^2) \) and \( \epsilon_{\gamma_1}(\theta) \) \( \text{iid} \sim N(0, \sigma_1^2) \) are mutually independent, and a flat prior is placed on \( \log(\sigma_1) \). Under this model, deformation data for both the flat cylinders
and the new pentagon are combined to inform the posterior distribution of $\alpha$. The posterior distribution of the local deformation feature for the new pentagon is derived based only on its data. Hamiltonian Monte Carlo is used to obtain 1000 posterior draws of $\alpha$, $\beta$, $\sigma_0^2$, and $\sigma_1^2$ after a burn-in of 500. We observe from the summary of the model fit in Figure 8 that our hierarchical model specification for $\delta_{\gamma_1}$ performs well in capturing pentagon deformation.

![Deformation and Model Fit of the New 3'' Pentagon](image)

Figure 8: Observed deformation (gray dots), and posterior predictive means (solid lines) and 95% central posterior predictive intervals (dashed lines) for points with $r_{\gamma_1}^{\text{nom}}(\theta) < 2.98$ in the new pentagon.
3.4 Application of the Learned Local Deformation Feature Model for an Irregular Polygon

The application of our Bayesian model building procedure on cylinders and a single new regular polygon clearly illuminates the essential structure of the local deformation feature for more general polygons. Specifically, consider a convex polygon with \( E \) edges and nominal radius function \( r_{\gamma_2}^{\text{nom}} : [0, 2\pi] \rightarrow \mathbb{R} \). As before, the edges of the polygon constitute natural blocks, and we define \( e : [0, 2\pi] \rightarrow \{1, \ldots, E\} \) as the function that returns the block level for each \( \theta \). We also define \( m : [0, 2\pi] \rightarrow [0, 2\pi] \) as

\[
m(\theta) = \arg\min_{t : e(t) = e(\theta)} r_{\gamma_2}^{\text{nom}}(t),
\]

and the clusters \( \Theta_1 = \{\theta \in [0, 2\pi] : \theta > m(\theta)\}, \Theta_2 = \{\theta \in [0, 2\pi] : \theta \leq m(\theta)\} \). The previously learned local deformation feature model is then extended to \( r_{\gamma_2}^{\text{nom}}(\cdot) \) as

\[
\delta_{\gamma_2}(\theta | \beta) = \sum_{k=1}^{2} \mathbb{I}(\theta \in \Theta_k) \delta_{\gamma_2,k}(\theta | \beta_{e(\theta),k}),
\]

with

\[
\delta_{\gamma_2,k}(\theta, | \beta_{e(\theta),k}) = \beta_{e(\theta),0} + \beta_{e(\theta),k,1} \left\{ r_{\gamma_2}^{\text{nom}}(\theta) - r_{\gamma_2}^{\text{nom}}(m(\theta)) \right\} b_{e(\theta),k}.
\]

Finally, we place a hierarchical model on the parameters in \( \beta \), and weakly informative priors on \( b_{e(\theta),1} \) and \( b_{e(\theta),2} \) as before.

Armed with this general local deformation feature, we can fit the deformation model using data from both the previously manufactured cylinders and a newly manufactured polygon. A polygon does not necessarily have a circumcircle, and so we instead use its minimum bounding circle for the global deformation feature. Thus, for a polygon with
nominal radius function $r_2(\cdot)$ and a minimum bounding circle of radius $\gamma_0$, its deformation model is specified as

$$\Delta^{\text{obs}}_{r_2}(\theta) = \delta_{\gamma_0}(\theta|\alpha) + \delta_{r_2}(\theta, \beta) + \epsilon_{r_2}(\theta),$$

where $\delta_{\gamma_0}(\theta|\alpha)$ is as defined as in (2), $\delta_{r_2}(\theta, \beta)$ is as defined in (7), and $\epsilon_{r_2}(\theta) \sim \text{N}(0, \sigma^2_{\epsilon})$. The priors for $\alpha$ and $\sigma^2_{\epsilon}$ are specified as before.

To illustrate the general utility of our learned local deformation feature model, consider the new irregular polygon displayed in Figure 9(a). Our model’s fit for this shape is summarized in Figure 9(b). We observe that our learned local deformation feature model performs well in capturing the new polygon’s deformation profile, especially in light of the fact that our model specification was based on just three cylinders and one regular polygon.

This case study also serves to highlight the differences between a learned local deformation feature model and a model obtained by more prescriptive approaches, which is constructed without reference to any data of a new shape. For example, Figure 10 compares the pre-specified sawtooth local deformation feature model drawn from the approach of Huang et al. (2014b), and our learned local deformation feature model, for the previous regular pentagon and irregular polygon. This figure suggests that pre-specified sawtooth functions may enjoy a limited scope of application for new shapes, and that the learned local deformation feature model obtained from our procedure is more targeted and appropriate for the broad class of new shapes. Also, the use of the minimum nominal radius for an edge in equation (8) provides a meaningful interpretation for our local deformation feature model parameters, which is not the case for models obtained from a prescriptive approach. The trade-off is that our method requires data on at least one new shape from this class, whereas a prescriptive approach does not.
Figure 9: (a) A new irregular polygon (solid line) and its minimum bounding circle (dashed line) of size $\gamma_0 = 1''$. (b) Observed deformation (gray dots), and posterior predictive means (solid line) and 95% central intervals (dashed lines), for the new polygon.

### 3.5 Application of the Learned Local Deformation Feature Model for the Straight Edges in a More General Shape

The previously learned local deformation feature model is not limited to regular and irregular polygons. Indeed, we have by inspection of equation (8) that it is immediately applicable to the straight edges in a shape. As a broad class of shapes are composed using various combinations of straight and curved edges, this application of our Bayesian model building procedure effectively reduces the problem of deformation modeling for such shapes under resource constraints.

To illustrate this point, we fit our deformation model to a shape that consists of four straight edges and one curved segment. This specific shape was constructed by adding the
Figure 10: (a) Pre-specified local deformation feature models for two polygons drawn from the work of Huang et al. (2014b). (b) Our learned local deformation feature models.

compensation plan in Figure 11(a) to a regular pentagon of size $1''$. The resulting nominal radius function $r_{\gamma_3}^{\text{nom}}(\cdot)$ for this new shape has one curved segment for $3\pi/2 - \pi/5 < \theta < 3\pi/2 + \pi/5$ (Figure 11(b)). The observed deformation for this shape, defined as

$$\Delta_{\text{obs}} r_{\gamma_3}(\theta) = r_{\gamma_3}^{\text{obs}}(\theta) - r_{\gamma_3}^{\text{nom}}(\theta),$$

is in Figure 12. As in the previous analyses, we fit the general deformation model simultaneously to the three cylinders and this new shape. The resulting fit is summarized in Figure 12. We observe that our deformation model performs well for the four straight edges, and does not provide a good fit for points on the curved segment. This corresponds to the fact that our local deformation feature model was learned from a single new shape consisting only of straight edges. As such, its scope of application includes straight edges,
Figure 11: (a) A compensation plan applied to a regular pentagon of size 1'' to yield a shape with four straight edges and one curved segment. (b) The curved segment (solid line) of the resulting shape, represented with Cartesian coordinates. For comparison, a straight edge is plotted as the dashed line.

but not necessarily curved segments, in new shapes. Learning a local deformation feature model for curved segments requires the application of our Bayesian procedure on at least one new shape with curved segments. In any case, this case study illustrates that the local deformation feature derived from our Bayesian model building procedure based on flat cylinders and a single regular pentagon persists for new shapes with similar features as our previously manufactured shapes.
Figure 12: Observed deformation (gray dots) and model fit for the new free-form shape. Solid lines denote the posterior predictive means, and dashed lines the 95% central posterior predictive intervals, of deformation.

4 Conclusion: Bayesian Model Building and Dynamic Recalibration in 3D Printing

Three-dimensional printing has created a paradigm shift in shape analysis and quality control, in the sense that small samples of data on distinct classes of shapes are all that are available for model building. We developed a Bayesian model building methodology that effectively addresses this complication in three steps. The first step is to use connections between distinct shapes, as postulated, for example, under the cookie-cutter framework, so as to extract information on a modular deformation feature for a newly manufactured
shape based on inferences drawn from previously manufactured and different shapes. This information was derived by means of a Bayesian discrepancy measure, which accounts for uncertainty in the shared, global deformation feature, and enables the illumination of a hierarchy of deformation features in the remaining two steps. Second is to identify and model systematic trends in the deformation feature based on its extracted information such that the specified deformation feature is directly applicable to a broad class of new shapes with similar features. The use of Bayesian statistics provides an advantage here because the posterior distribution of the global deformation feature model parameters provide uncertainty measures that are immediately applicable to facilitate testing of trends in the local deformation feature. The final step is to specify a hierarchical structure on the new deformation feature model parameters across different parts of the shape so as to make full use of the small sample of data for inference and prevent overfitting. Our case studies of flat cylinders, polygons, and a free-form shape demonstrate how this Bayesian model building methodology enlightens the accelerated and efficient specification of deformation models for a broad class of new shapes that share similar features. This is especially important for complex shapes, in which case a local deformation feature model cannot be conceived \textit{a priori}, and hence prescriptive approaches may not yield success. Furthermore, our case studies illustrate how data on different shapes can be used simultaneously to infer the parameters of the resulting model. This is a significant feature of our approach, and directly corresponds to combining all available data to more precisely predict deformation.

It is important to note that our methodology is not limited to a specific 3D printing technology. In principle, it can abstract the essential features of a large variety of technologies, and thus is widely applicable. There also exists the potential to reveal cross-cutting scientific and engineering principles by applying our approach to different settings, printers, and materials.
Our methodology illuminates the path to Bayesian dynamic recalibration of poorly specified local deformation features or ineffective compensation plans with little further experimentation. We observe from the case study in Section 3.5 that, if an initial specification of a deformation model and associated compensation plan does not sufficiently reduce deformation, the manufactured shape is not a complete loss because it still contains useful information for updating the deformation model and compensation plan. Indeed, after a new shape, compensated or uncompensated, has been printed, we can use different types of discrepancy measures in the first step of our general Bayesian methodology to directly learn from the single new shape and previous (distinct) shapes how to refine the prior conception of the shape’s deformation model and corresponding compensation plan for improved quality control in the future. A successful application of this step will yield smart 3D printing with the potential of immediate practical application. Such a rapid and effective dynamic between deformation modeling and compensation plan development will enable a closed loop that addresses the goal of low-cost, high-confidence prediction of shape geometry, to further promote 3D printing as a high-quality manufacturing technology. Ultimately, our Bayesian model building methodology can play an important role for statistical shape analysis more broadly in quality control settings characterized by small samples of data on distinct shapes with partially shared features.

Appendix: Prior Specification for Global Deformation Feature Model Parameters

We place flat priors on \( \alpha_{0,U}, \alpha_{0,L}, \alpha_{1,U}, \alpha_{1,L}, \) and \( \log(\sigma_0) \), and specify

\[
a_{0,U}, a_{0,L} \sim N(1, 2^2), \quad a_{1,U}, a_{1,L} \sim N(1, 1^2),
\]
\[
\log \left( \frac{0.5 + x_{0,U}}{0.5 - x_{0,U}} \right), \quad \log \left( \frac{0.5 + x_{0,L}}{0.5 - x_{0,L}} \right) \sim N(0, 1^2), \quad \text{and} \]
\[
\log \left( \frac{\psi_{U}/\pi}{1 - \psi_{U}/\pi} \right), \quad \log \left( \frac{\psi_{L}/\pi}{1 - \psi_{L}/\pi} \right) \sim N(0, 1^2).
\]

Our priors for \(a_{0,U}, a_{0,L}, a_{1,U}\) and \(a_{1,L}\) are based on the reasoning of Huang et al. (2015, p. 436). As we can assume that \(0 < x_{0,U} + 0.5, x_{0,L} + 0.5 < 1\), we specify weakly informative priors (Gelman et al., 2008) on logistic transformations of \(x_{0,U} + 0.5, x_{0,L} + 0.5\). A similar logic motivated the prior specifications on \(\psi_{U}\) and \(\psi_{L}\).

References


