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Manufacturing quality prediction using smooth spatial variable selection estimator with applications in aerosol jet® printed electronics manufacturing

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ABSTRACT

Additive manufacturing (AM) has advantages in terms of production cycle time, flexibility, and precision compared with traditional manufacturing. Spatial data, collected from optical cameras or *in situ* sensors, are widely used in various AM processes to quantify the product quality and reduce variability. However, it is challenging to extract useful information and features from spatial data for modeling, because of the increasing spatial resolutions and feature complexities due to the highly diversified nature of AM processes. Motivated by the aerosol jet® printing process in printed electronics, we propose a smooth spatial variable selection procedure to extract meaningful predictors from spatial contrast information in high-definition microscopic images to model the resistances of printed wires. The proposed method does not rely on extensive feature engineering, and has the generality to be applied to a variety of spatial data modeling problems. The performance of the proposed method in prediction and variable selection through simulations and a real case study has proven to be both accurate and easy to be interpreted.

1. Introduction

The challenges in Additive Manufacturing (AM) processes relate to product quality quantification, monitoring and control, all of which impede its broader application. Extensive efforts have been made in recent years on quality modeling of AM using *in situ* process information (Rao *et al.*, 2016). Among these efforts, spatial data has been widely collected and analyzed for various AM processes (Huang *et al.*, 2015). However, due to the increase in spatial resolution and feature complexity, it is still a challenge to efficiently use spatial data in AM quality engineering (Schabenberger and Gotway, 2017). More investigations are thus needed to improve the modeling and interpretation of spatial data in AM quality control. In this article, we focus on quality modeling of additive-manufactured electronics with spatial data to reflect process conditions.

Along with this direction, our research is motivated by an aerosol jet® printing (AJP) process, which is a direct write type of AM for flexible electronics printing. The basic procedures of the AJP process are as follows:

1. Nanoparticle silver ink is atomized into droplets (mists) by an atomizer.
2. The mist is delivered by carrier gas to the nozzle.
3. The mist is pushed out of the nozzle at a high velocity onto the surface that is being printed.

More details of the process can be found in Sun *et al.* (2017).

In the AJP process, high-resolution microscopic images are taken of the surfaces of the printed electronics, as shown in Figure 1(a), as an indirect measure of their quality. As the microscope takes the images in a non-contact manner, it can prevent potential damage and human errors in measurements caused by traditional contact-based measuring tools, such as multi-meters (Mahajan *et al.*, 2013). These microscopic images, reflecting the distribution of the silver inks on the printed electronics, have been proven to strongly correlate with the resistance and other electronic properties of the investigated samples (Sun *et al.*, 2017).

However, there is lack of efficient and systematic ways to identify interpretable features from the raw images to model electronic properties. Instead of performing the complex engineering-driven feature extractions requiring domain knowledge as shown on the right of Figure 1(b), we intend to use a spatially correlated predictor that is generated from an image pixel or mesh to directly predict the quality response, as shown on the left of Figure 1(b). Here, a mesh consists of multiple pixels from an area in an image with its intensity calculated by the mean intensity of all pixels in the mesh. Specifically, we focus this study on generation and variable selection methods for spatially correlated predictors (i.e., images in the AJP process) to help identify interpretable features for predicting the resistance properties of conducting wires. Note that wires with missing segments and infinite resistances are treated as outliers and removed from the modeling study.
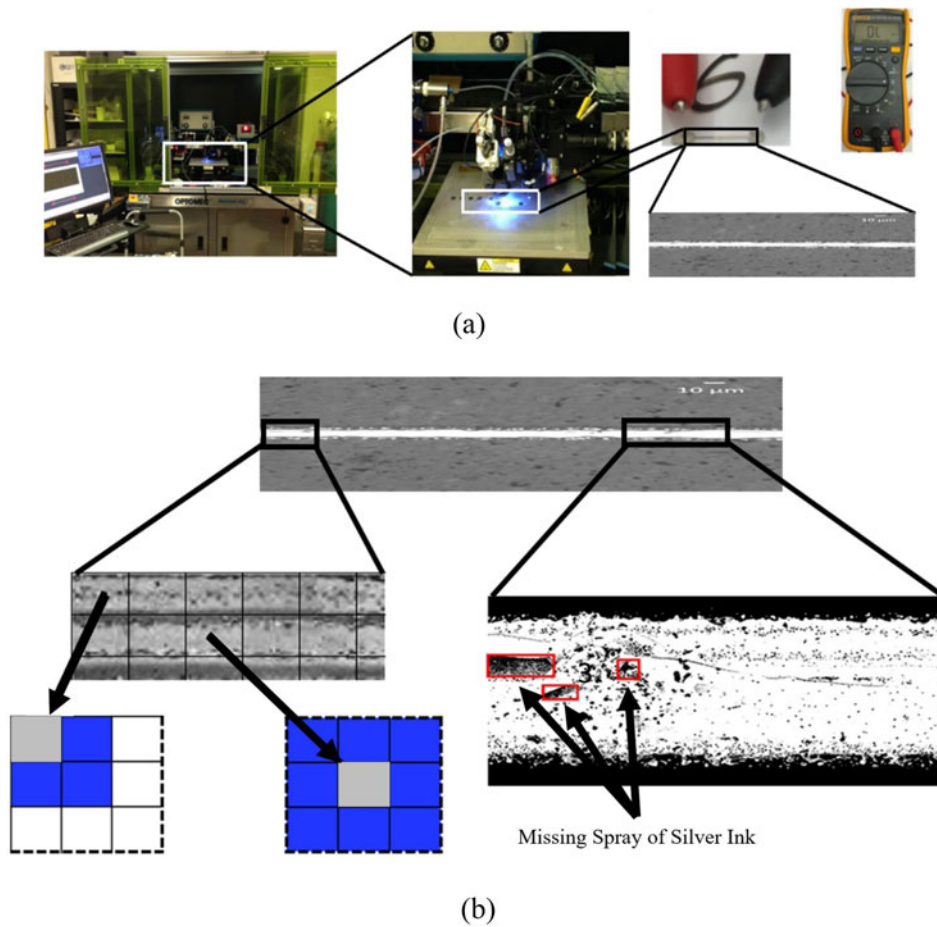
Figure 1. (a). Optomec aerosol jet® system (left), the printing process (middle), and the resistance measurement on printed electronics using a multi-meter and a microscopic image of the printed electronics (right) and (b) two distinct ways of generating variables for resistance prediction: spatial predictor extraction with an example of contrast between a pixel and its 8-Connected neighborhoods (defined in Adams and Bischof (1994) (left) and engineering-driven feature extraction (Sun et al., 2017) (right).

In the literature, there are various papers that use spatially correlated predictors for variable selection and modeling. Note that these methodologies are different from spatial statistics, which typically emphasize the modeling and analysis of spatially correlated responses (Ripley, 2005). Here our focus is on "spatial-data-in-scalar-out" types of regression, which are also known as the "scalar-on-image" (Kang et al., 2016) regressions for image data. Two of the most commonly used methodologies are feature-extraction-based modeling, and direct modeling (e.g., treat the intensity of each pixel as a predictor). For feature-extraction-based modeling, wavelet analysis (Bukkapatnam et al., 1999), homologous features (Li et al., 2015), and Fourier transforms (Li, Ledo, Delgado, Cerrada, Pacheco, Cabrera, Sánchez, and de Oliveira, 2017), etc., can be used to extract features from raw spatial data. Then, regression models can either use the extracted features as input variables or employ feature reduction (Bai et al., 2018) before performing variable selection and prediction. Kernel-based models are also widely adopted, such as kernel-ridge regression (Vovk, 2013), relevance vector regression (Zheng and Fang, 2015), etc. The kernel-based model transforms the original data sets into dual forms of various kernel spaces, in order to reduce the modeling complexity and change the model linearity for better performance. One potential drawback of the methods mentioned above is that sufficient domain knowledge on the corresponding manufacturing processes and a large amount feature engineering are often needed to generate high-quality predictors. As a result, a strategy to directly select individual variables without complex feature extraction procedures or kernel function selection is more useful to directly identify important features, which is called the direct modeling method in this article.

For the direct modeling method, popular approaches include tensor regressions (Li et al., 2013), matrix regression (Zhou and Li, 2014), deep learning (Chen et al., 2014), Gaussian Process (GP) models (Kang et al., 2016), which have been re-engineered to handle "scalar-on-image" regression based on traditional GP models (Colosimo et al., 2015), etc. However, many tensor and matrix regressions are usually built under the assumption of low-rank approximations (Zhou and Li, 2014), which might not always be adequate for the spatial data sets collected in AM processes (Sun et al., 2017). The models used in deep learning, such as convolutional neural network (CNN), are relatively complex and require large sample sizes of input data (Luo, 2017). However, in a highly flexible AM process, the sample size can become very small (e.g., measured at most in tens or hundreds), since AM often produces a "one-of-a-kind" design of products to satisfy personalized needs.

Furthermore, complex model structures produced by deep learning can be difficult to use to generate interpretable features for further diagnosis on product quality (Lou *et al.*, 2012). The use of GP models also involves high computational costs and large sample size requirements, making it difficult for data modeling with a large number of variables and limited sample sizes in AM processes (Tripathy *et al.*, 2016).

In this article, we focus on using spatial data to study the resistance variation of printed wires due to missing ink spray defects (black pinholes/regions in the image of Figure 2(b)). It has been shown that an increase in the number of such defects significantly increases the resistance of a printed wire (Zhao *et al.*, 2012). It is worth mentioning that, not only in the AJP process, various other printing processes for flexible electronics, including flexographic printing (Krebs, 2009), inkjet printing (Haverinen *et al.*, 2010), and gravure printing (Kang *et al.*, 2012), also suffer from quality issues due to missing ink spray defects, such as short circuits, high energy loss, etc. In this article, we propose to generate and select spatial predictors that directly allow accurate quality prediction and good interpretability. The proposed approach is to encourage similar-but-non-identical effects among neighborhood predictors, pursuing the smoothness among neighborhood parameters during variable selection. The underlying motivation is that predictors in a neighborhood are spatially correlated, and thus would take similar roles (e.g., either all be significant or insignificant) in affecting the response. Thus, the parameter value changes among spatially adjacent predictors are expected to be smooth. For example, in microscopic images of printed wires, the parameter values would gradually decay as the corresponding predictors are far away from the defect regions, which are strongly associated with the response. We refer to such a phenomenon as the *neighborhood effect*. Such an effect is inherent to many spatially adjacent predictors in spatial data modeling (Kang *et al.*, 2016). In the AJP process, the spatial contrast information generated from the microscopic images can directly predict the resistances of conducting wires through the proposed spatial modeling framework.

For predictor generation, three different types of spatial contrast information (Adams and Bischof, 1994) will be used to form spatial predictors: (i) contrast (difference) between each mesh's intensity and the overall image's mean intensity; (ii) contrast (difference) between each mesh's intensity and its 8-Connected neighborhood meshes' mean intensity; and (iii) contrast (difference) between each mesh's intensity and the largest row-wise mean intensity among the image. Comparing with the past AJP-related quality quantification work (Sun *et al.*, 2017), an advantage of using spatial predictors is that it requires neither heavy feature engineering nor manually labeled quality indices (e.g., silver ink over-spray) for product quality quantification. An example of spatial predictors from the microscopic images is shown in Figure 2, which is motivated by the work of Adams and Bischoff (1994) to reflect local intensity variation.

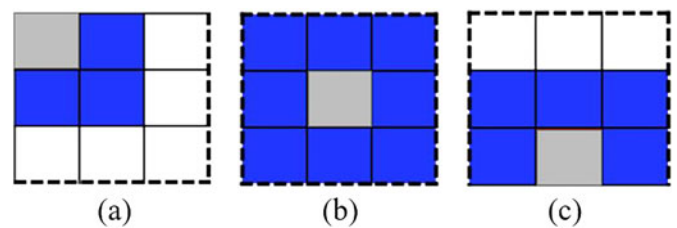In summary, we remark that the proposed model, Smooth Spatial Variable Selection (SSVS), is easy to

Figure 2. The 8-Connected neighborhoods of the underlying mesh are its surrounding meshes.

interpret since the spatial predictors are directly generated from the spatial data, such as the contrast information among pixels. Both one-dimensional (1-D) and two-dimensional (2-D) simulations show that SSVS better identifies inherent structures among model parameters, by encouraging their smoothness. The case study on a real system shows that given the highly personalized nature of AM processes, SSVS under small training sample sizes offers smaller prediction errors on testing data and yields meaningful variable selection results. This gives SSVS the potential to be widely adopted for quality modeling in various AM processes and spatial data modeling problems.

The remainder of this article is organized as follows. In Section 2, the proposed modeling framework, SSVS, and the estimation algorithm are introduced. In Section 3, simulation studies for SSVS comparing with benchmark models are introduced. The benchmark models in this research mainly include Lasso, fused Lasso, and matrix regression, where Lasso is known for its variable selection under sparse model parameter spaces, fused Lasso and matrix regression are known for their ability to recover certain types of model parameter structures. Details of these models and their comparisons with the proposed method will be discussed later. Section 4 presents a case study that uses SSVS to investigate the AJP process. Finally, Section 5 summarizes the proposed methodology and discusses future work.

2. Smooth spatial variable selection for models with spatial predictors

2.1. Model formulation

Without loss of generality, we consider a linear regression between a single response variable y, such as the resistance of a wire, and 2-D spatial predictors

$$\mathcal{X} = \begin{pmatrix} \mathcal{X}_{1,1} & \cdots & \mathcal{X}_{1,m} \\ \vdots & \ddots & \vdots \\ \mathcal{X}_{l,1} & \cdots & \mathcal{X}_{l,m} \end{pmatrix},$$

a $l \times m$ matrix, where each predictor can correspond to a pixel or a mesh location for microscopic images of conducting wires. Given that each predictor in the matrix $\mathcal{X}$, such as $\mathcal{X}_{i,j}$, is spatially located by its index (i, j) in a 2-D space, we can vectorizie $\mathcal{X}$ and the corresponding $l \times m$ model parameter matrix B without losing their spatial information. Specifically, $tr(\mathcal{X}^T B)$ defines the summation of the pair-wise multiplication of the corresponding elements in matrices $\mathcal{X}$ and B. Therefore, if one vectorizies $\mathcal{X}$ and B, by appending

the columns sequentially into $x = (x_{1,1}, ..., x_{l,m})^T$ and $\beta = (\beta_{1,1}, ..., \beta_{l,m})^T$, into $(lm) \times 1$ vectors, each pair of elements in $\mathcal{X}$ and B to be multiplied remain unchanged. As a result, the summation of pair-wise multiplication defined by $tr(\mathcal{X}^T B)$ remains equivalent to performing vector-wise multiplication $x^T \beta$. Thus, we can present the 2-D model formulation in a 1-D format:

$$y = tr(\mathcal{X}^T B) + \varepsilon = x^T \beta + \varepsilon, \tag{1}$$

where $\varepsilon \sim N(0, \sigma^2)$ is an independent and identically distributed (i.i.d) error term. It should be noted that such an indexing of predictors can be easily generalized to data organized in a higher-dimensional format, such as three-dimensional (3-D) colored image data and even four dimensional spatial-temporal video data (Yan et al., 2015), where the neighborhood effect can be enforced among spatially adjacent model parameters.

In order to conduct the selection of variables for model (1), various methods are proposed in the literature, such as Lasso (Tibshirani, 1996), which is a commonly used method, but not designated for spatial variable selection (Tibshirani et al., 2005). Tibshirani et al. (2005) introduced fused Lasso to penalize the difference between model parameters, and this encourages the smoothness of variables. The applications of fused Lasso for 2-D spatial data sets are discussed in the work of generalized Lasso (Tibshirani and Taylor, 2010), which can enforce model parameter structures using designated penalty matrices. Both fused Lasso and generalized Lasso mainly focus on piece-wise constant variable selection, that is, the similarity of two adjacent model parameters is encouraged by penalizing their differences in the model. Furthermore, the generalized Lasso does not enforce the overall sparsity of model parameters, which is not suitable for high-dimensional modeling under the spars-

Furthermore, the magnitudes of $\beta_{o,u}$ gradually decay (less significant) as the locations of the corresponding predictors become further away from $x_{i,j}$. The proposed SSVS does not only enforce the similarity among neighborhood model parameters, but also makes the similarity tunable through adjusting the value of r in model estimation (see Section 2.2). The larger the value of r considered for the variable selection, the smoother the changes among neighborhood parameters.

2.2. The smooth variable selection estimator

Suppose that $y = (y_1, ..., y_n)^T$ is an $n \times 1$ response vector observed for the y in model (1), containing resistances of n printed wires, and

$$X = \begin{pmatrix} x_{1,(1,1)} & \cdots & x_{1,(l,m)} \\ \vdots & \ddots & \vdots \\ x_{n,(1,1)} & \cdots & x_{n,(l,m)} \end{pmatrix}$$

is a $n \times lm$ predictor matrix observed for x in model (1), containing the values of the spatial predictors from n microscopic images of printed wires. By incorporating SSVS, the model estimation in model (1) can be solved by minimizing:

$$\min \frac{1}{2}||y - X\beta||_2^2 + \lambda_1 ||\beta||_1 + \lambda_2 ||S\beta||_1, \tag{2}$$

where

$$S = \begin{pmatrix} S_{(1,1),(1,1)} & \cdots & S_{(1,1),(l,m)} \\ \vdots & \ddots & \vdots \\ S_{(l,m),(1,1)} & \cdots & S_{(l,m),(l,m)} \end{pmatrix}$$

is an $lm \times lm$ weight matrix with its component being

$$S_{(i,j),(o,u)} = \begin{cases} -\dfrac{\exp\left(-\sqrt{(i-o)^2 + (j-u)^2}\right)}{\sum_{z=1}^{r} \exp(-z)} & \forall (o,u) \in \left\{\sqrt{(i-o)^2 + (j-u)^2} \leq r, i \neq o, j \neq u\right\} \\ 0 & \forall (o,u) \in \left\{\sqrt{(i-o)^2 + (j-u)^2} > r, i \neq o, j \neq u\right\} \\ -\sum_{o \neq i}\sum_{u \neq j} S_{(i,j),(o,u)} & o = i, u = j \end{cases}.$$

ity assumption of model parameters. In the spirit of both fused Lasso and generalized Lasso, we propose SSVS to encourage the similarity and smoothness of spatially adjacent model parameters. For elaboration, we denote the parameter of a predictor $\mathcal{X}_{i,j}$ in $\mathcal{X}$ as $\beta_{i,j}$, and define the r-neighborhoods of $\beta_{i,j}$ as the set of parameters $\left\{\beta_{o,u} : \sqrt{(i-o)^2 + (j-u)^2} \leq r\right\}$, where the distance of any two parameters is measured by the Euclidean distance. The SSVS encourages that if the value of $\beta_{i,j}$ is non-zero (i.e., the i,jth predictor is important), the parameters $\beta_{o,u}$ in its r-neighborhoods also tend to have non-zero values.

Here the smoothness is achieved by penalizing the difference between weighted parameter $S_{(i,j),(i,j)}\beta_{i,j}$, and the sum of its weighted neighborhood parameters $\sum_{o \neq i}\sum_{u \neq j} S_{(i,j),(o,u)}\beta_{o,u}$, which are no more than a distance r away from $\beta_{i,j}$ measured in terms of the Euclidean distance. The weights are determined by the normalized exponential distance weighting function

$$\frac{\exp\left(-\sqrt{(i-o)^2 + (j-u)^2}\right)}{\sum_{z=1}^{r} \exp(-z)},$$

which ensures that the weight on each neighborhood parameter is in [0,1] with the denominator/normalizing factor

$\sum_{z=1}^{r} \exp(-z)$. The same r is considered for all predictors when estimating the model parameters. It is important to point out that when there is only one neighborhood considered ($r = 1$) for the estimator, $||S\boldsymbol{\beta}||_1$ only penalizes the differences of two consecutive model parameters, which are one distance away from each other. Hereafter, SSVS with only one neighborhood is the same as the fused Lasso approach. Also, for spatial predictors from image data, the matrix S can further enforce the smoothness on predictors arranged in irregular grids. For example, we can use the adjacency information, such as a 0-1 binary indicator, instead of 2-D Euclidean distances among predictors to calculate $S_{(i,j),(o,u)}$.

2.3. Parameter tuning and model estimation

In model (2), we consider using the Extended Bayesian Information Criterion (EBIC) (Chen and Chen, 2012) to select tuning parameters r, λ_1, and λ_2. Here, EBIC is used because traditional model selection criteria, such as the Bayesian information criterion (Schwarz, 1978) and the Akaike information criterion (Akaike, 1998) do not have consistent and satisfying model selection when the number of variables is much larger than the sample size. EBIC leverages both the number of unknown parameters to estimate and the resulted model complexity for model selection. As a result, it has been shown that EBIC can yield more accurate and consistent modeling performance for high-dimensional modeling under small sample sizes (Chen and Chen, 2012).

The objective function in model (2) is a quadratic function, which can be solved by standard quadratic programming algorithms, such as Newton's method and the interior point method. However, for a modeling problem with a high dimension of predictors, taking the second derivation required by some optimization methods is computationally intensive. To address this issue, we adopted the split Bregman algorithm, which is a type of alternating direction method of multipliers algorithm, which will quickly converge under l_1 norm (Ye and Xie, 2011).

Ye and Xie (2011) proposed a general framework for solving the constrained optimization problem:

$$\min \ V(\boldsymbol{\beta}) + \lambda_1 ||\boldsymbol{a}||_1 + \lambda_2 ||\boldsymbol{b}||_1,$$

$$\text{subject to : } \boldsymbol{a} = \boldsymbol{\beta}, \boldsymbol{b} = S\boldsymbol{\beta},$$

which has the augmented Lagrangian function of the form of

$$L(\boldsymbol{\beta}, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{u}, \boldsymbol{v}) = V(\boldsymbol{\beta}) + \lambda_1 ||\boldsymbol{a}||_1 + \lambda_2 ||\boldsymbol{b}||_1 + \langle \boldsymbol{u}, \boldsymbol{\beta} - \boldsymbol{a} \rangle$$
$$+ \langle \boldsymbol{v}, S\boldsymbol{\beta} - \boldsymbol{b} \rangle + \frac{\mu_1}{2} ||\boldsymbol{\beta} - \boldsymbol{a}||_2^2 + \frac{\mu_2}{2} ||S\boldsymbol{\beta} - \boldsymbol{b}||_2^2,$$

where $V(\boldsymbol{\beta})$ is a convex function, $\langle \cdot, \cdot \rangle$ is the inner product of two vectors, $\boldsymbol{u}$ and $\boldsymbol{v}$ are dual variables corresponding to the two linear constraints, and μ_1 and μ_2 are positive augmented Lagrangian parameters controlling the speed of optimization. The convergence of the algorithm is guaranteed.

3. Simulation studies

In the simulation studies, we consider two simulations, one with a 1-D format of predictors and one with a 2-D format of predictors to systematically evaluate the prediction and variable selection performance of the proposed SSVS estimator. The SSVS estimator will be compared with three benchmark models, including Lasso, fused Lasso, and nuclear-norm-based matrix regression (for the 2-D dataset). Other models, such as CNN and GP models, were not selected as benchmark models, due to their large sample size requirements in model estimation (Tripathy et al., 2016).

3.1 A 2-D simulation study of SSVS

We created a simulation study with 2-D spatial predictors to illustrate the benefits of SSVS on 2-D data sets. To ensure the generality of the simulation results and showcase the importance of having a smoothness-tunable variable selection process, we assumed that model parameters, and the mean values and covariance of the predictors all had varying spatial correlations across different replications, respectively. Furthermore, we intentionally designed the generation of the parameter smoothness to make the decay pattern of model parameters different from the weights assigned in the smoothing matrix S of Equation (2). As a result, a random decay pattern on model parameters will be chosen for each replication of the simulation.

To generate the spatially correlated covariance of the spatial predictors, we defined the covariance between variable $x_{i,j}$ and $x_{o,u}$ on a 2-D space with an exponential decay function

$$\sigma_{i,j;o,u} = \text{cov}(x_{i,j}, \ x_{o,u}) = \frac{1}{\tau^{\sqrt{(i-o)^2 + (j-u)^2}}},$$

where the covariance shrinkage parameter (τ) had a value of five. In this way, the covariance of variables, which were spatially close to each other, had larger correlations. Similarly, to generate the means of variables, we first randomly selected five predictors as the centers of the defects, which were bounded by radius φ following a discrete uniform distribution of $\{3, 4, 5\}$ to simulate defects with different sizes. Then the spatially correlated mean of each predictor within the defect area having the center at predictor $x_{i,j}$ was defined as,

$$\mu_{o,u} = 255 \left(1 - \frac{1}{\omega^{\sqrt{(i-o)^2 + (j-u)^2}}} \right) \ \forall \ (o,u)$$

$$\in \left\{ \sqrt{(i-o)^2 + (j-u)^2} \leq \varphi, o \neq i, u \neq j \right\},$$

where the shrinkage parameter (ω) followed a discrete uniform distribution of $\{1.1, 1.2, 1.3, 1.4, 1.5\}$. Here, we define defect areas, which have significantly lower intensities in microscopic images (Figure 1), as the regions that were not uniformly sprayed with silver ink in the printing process. Different values of ω can be used to simulate defect areas with different intensity shrinkage rates from the centers of the defects. For predictors outside of the defect area, the means were simply defined as
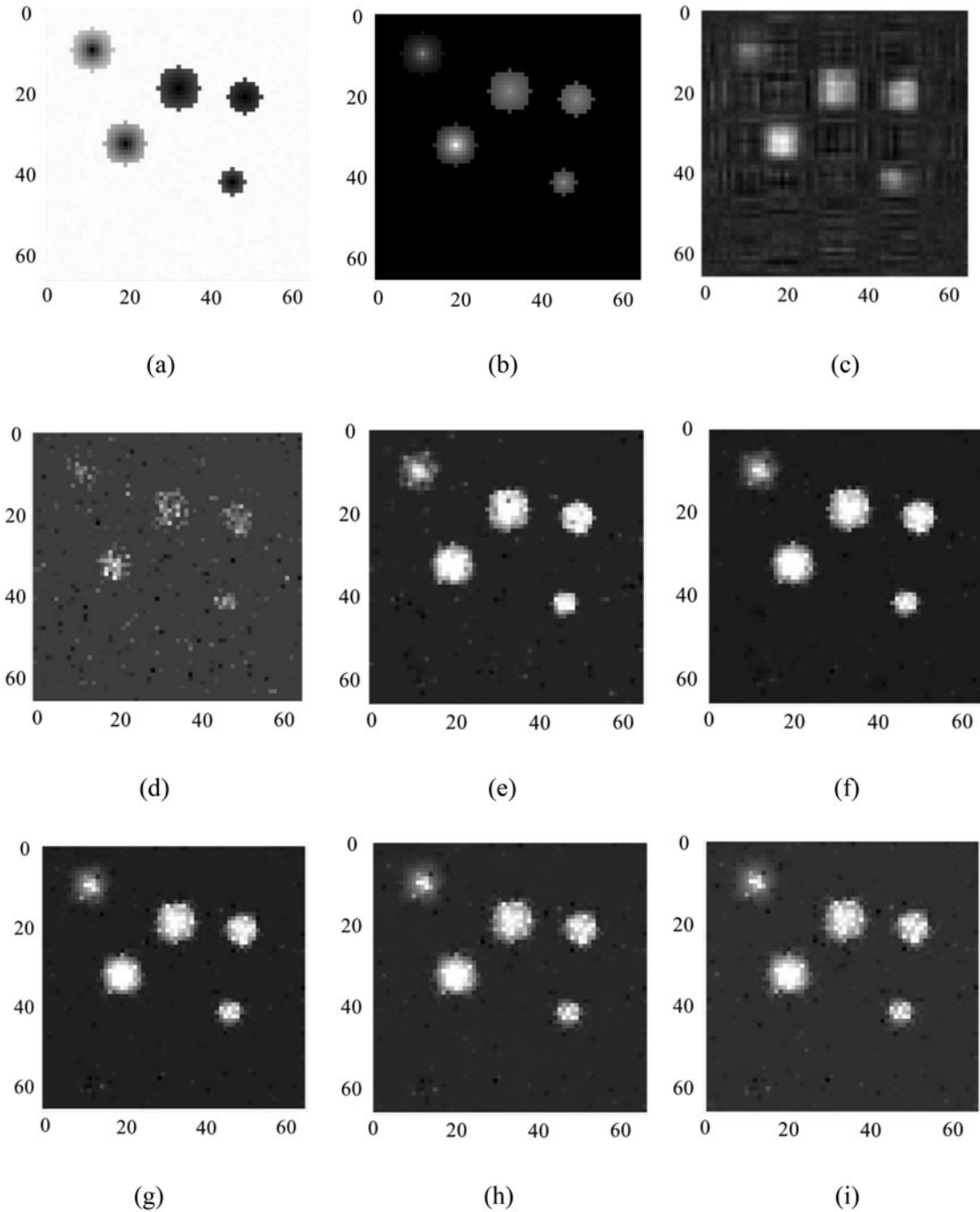
Figure 3. (a) An example of 2-D predictors simulated, (b) the 2-D model parameters simulated (underlying true parameters), (c) variable selection result using matrix regression, (d) variable selection result using Lasso, (e)-(i) variable selection result using SSVS considering one to five neighborhoods (two being the optimal).

$$\mu_{o,u} = 255 \; \forall \; (o,u) \in \left\{ \sqrt{(i-o)^2 + (j-u)^2} > \varphi, o \neq i, u \neq j \right\}.$$

Such a mean value generation approach ensured that the means of predictors within defect areas, which were darker than non-defect areas, were assigned with values smaller than 255. For the means of predictors not within the defect areas, they were assigned with 255 (the largest value/brightest color in a gray-scale image). As result, each predictor $x_{o,u}$ within each image sample followed i.i.d. $N(\mu_{o,u}, \sigma_{i,j;o,u})$, with one defect area existing. We repeatedly used such

methods to generated image samples containing five defect areas selected previously.

To generate spatially correlated model parameters, we assumed that only predictors within the defect areas had non-zero values. Here, we used the same five predictors select previously as the centers of the five defect areas and the following equation was used to generate the parameters of variables within the defect areas

$$\beta_{o,u} = \frac{\gamma}{\omega^{\sqrt{(i-o)^2 + (j-u)^2}}} \; \forall \; (o,u) \in \left\{ \sqrt{(i-o)^2 + (j-u)^2} \leq \varphi, o \neq i, u \neq j \right\},$$

Table 1. Testing RMSE values over 100 replications for the 2-D simulation data set (standard errors in parenthesis).

	Benchmark Models			Proposed Model
	Matrix Regression	SSVS ($\gamma = 0$) / Lasso	SSVS ($\gamma = 1$) / Fused Lasso	SSVS ($\gamma = 2$)
RMSE	23.56 (<0.00)	33.32 (0.34)	11.07 (0.18)	**10.03 (0.12)**

Table 2. Average variable selection accuracies (ACCs) over 100 replications for the 2-D simulation data set (standard errors in parenthesis).

	Benchmark Models			Proposed Model
	Matrix Regression	SSVS ($\gamma = 0$) / Lasso	SSVS ($\gamma = 1$) / Fused Lasso	SSVS ($\gamma = 2$)
RMSEs	0.48 (<0.01)	0.89 (<0.01)	0.96 (<0.01)	**0.97 (<0.01)**
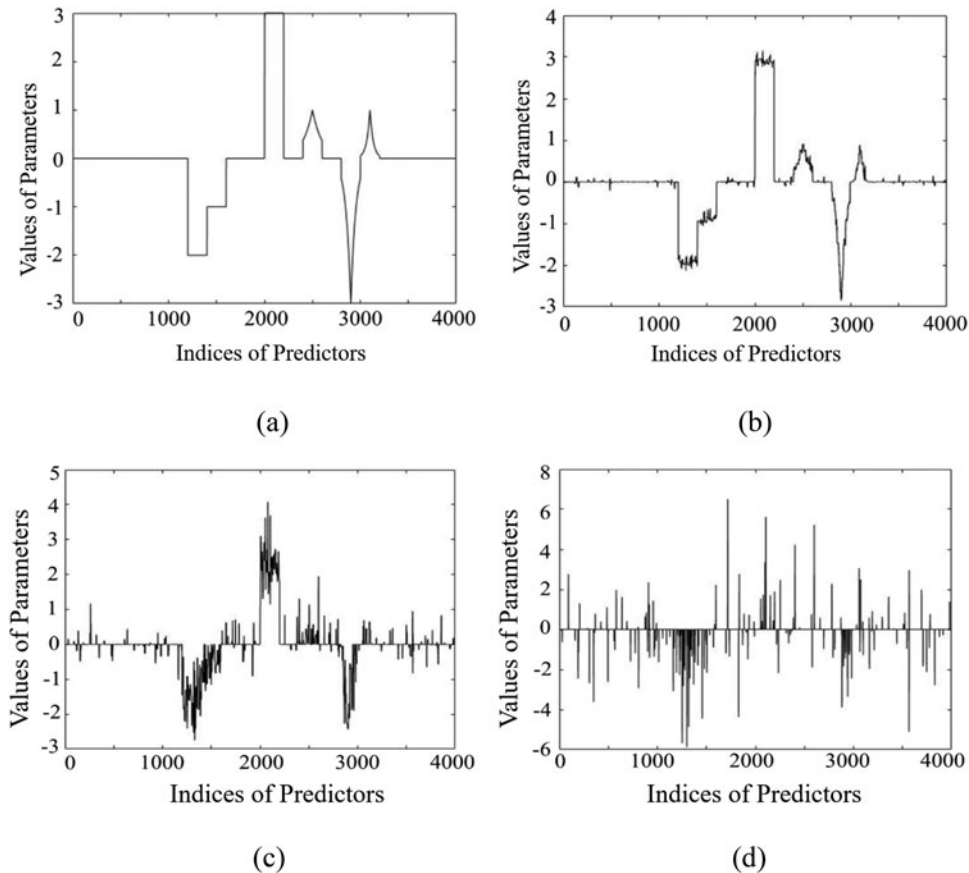
Figure 4. (a) True values of the simulated parameters, (b) the parameters learned considering more than one neighborhoods using SSVS' (c) the parameters learned considering one neighborhood using SSVS (fused Lasso). and (d) the parameters learned considering no neighborhood (Lasso).

where the defect center's parameter value (γ) followed a discrete uniform distribution of {1, 2, 3, 4, 5}. As the variable within the defect area was further away from the defect center, it had a smaller parameter value. For parameters outside of the defect areas, they were assigned with zeros

$$\left(\beta_{o,u} = 0 \ \forall \ (o,u) \in \left\{ \sqrt{(i-o)^2 + (j-u)^2} > \varphi, o \neq i, u \neq j \right\} \right).$$

Eventually, the response was generated based on model (1) with the values generated above and ε following i.i.d. $N(0, 1)$.

Similar to the simulation settings in Zhou and Li (2014), we used the above methods to generate 500 64 × 64 image samples with an example shown in Figure 3(a) to 3(i) and a set of 64 × 64 2-D model parameters shown in Figure 3(b).

To evaluate the consistency of the results, we simulated 100 replications for each simulation scenario. Within each replication, we randomly used 90% of the simulated samples as the training dataset and the remaining 10% as the testing dataset (Zeng et al., 2016). The tuning parameters were selected based on EBIC for Lasso and SSVS, and BIC for matrix regression (Zhou and Li, 2014). The simulation results including the testing data prediction accuracy in Root Mean Squared Error (RMSE) and the corresponding standard error (SE) values are presented in Table 1. The value shown in bold is the best result (smallest error) obtained from different models and SSVS achieved the lowest error with $r = 2$. The variable selection results are presented in Table 2 based on variable selection accuracies

Table 3. Average RMSE values over 100 replications for testing data in 1-D simulation studies.

		$\tau = 1.01$		$\tau = 1.05$	
p	Size of Neighborhoods for SSVS	$n = 40$	$n = 400$	$n = 40$	$n = 400$
4000	SSVS ($r = 0$) / Lasso	145.29 (8.48)	14.32 (0.67)	199.55 (9.07)	26.15 (1.12)
	SSVS ($r = 1$) / Fused Lasso	31.57 (2.38)	**1.42 (0.02)**	61.41 (4.04)	**1.48 (0.03)**
	SSVS ($r > 1$)	**30.49 ($r = 3$) (2.16)**	1.52 ($r = 3$) (0.03)	**55.23 ($r = 4$) (3.58)**	1.55 ($r = 2$) (0.03)
8000	SSVS ($r = 0$) / Lasso	342.21 (15.59)	33.15 (1.42)	327.54 (13.41)	64.95 (2.72)
	SSVS ($r = 1$) / Fused Lasso	185.84 (11.68)	**2.01 (0.04)**	229.56 (9.83)	**2.38 (0.05)**
	SSVS ($r > 1$)	**176.28 ($r = 4$) (10.57)**	2.11 ($r = 2$) (0.04)	**209.87 ($r = 5$) (9.61)**	2.54 ($r = 2$) (0.06)

Table 4. Average variable selection accuracies (ACCs) over 100 replications for the 1-D simulation dataset (standard errors in parenthesis).

		$\tau = 1.01$		$\tau = 1.05$	
p	Size of Neighborhoods for SSVS	$n = 40$	$n = 400$	$n = 40$	$n = 400$
4000	SSVS ($r = 0$) / Lasso	0.83 (0.01)	0.89 (<0.01)	0.83 (9.07)	0.89 (0.01)
	SSVS ($r = 1$) / Fused Lasso	0.96 (<0.01)	1.00 (<0.01)	0.92 (0.01)	1.00 (<0.01)
	SSVS ($r > 1$)	**0.97 ($r = 3$) (<0.01)**	**1.00 (*All r*) (<0.01)**	**0.93 (*All r*) (0.01)**	**1.00 (*All r*) (<0.01)**
8000	SSVS ($r = 0$) / Lasso	0.84 (<0.01)	0.88 (<0.01)	0.84 (<0.01)	0.88 (<0.01)
	SSVS ($r = 1$) / Fused Lasso	**0.87 (0.01)**	1.00 (<0.01)	0.82 (0.01)	1.00 (<0.01)
	SSVS ($r > 1$)	**0.87 ($r = 5$) (0.01)**	**1.00 (*All r*) (<0.01)**	**0.83 ($r = 5$) (0.01)**	**1.00 (*All r*) (<0.01)**

$$ACC = \frac{True\ Negative + True\ Positve}{Total\ Amount\ of\ Predictors}$$

and Figure 3. The modeling assumptions were validated by residual plots that are presented in the online supplementary materials.

From Table 1, Table 2, and Figure 3, it is clear that Lasso, which did not consider the neighborhood effect, performed the worst in prediction studies. It also had a large number of misdetections on significant model parameters (insignificant parameters misidentified as significant) during variable selection (Figure 3(d)). Furthermore, we can see that the matrix regression method, which relied on low-rank approximation, did not recover the parameter structures as good as did SSVS in this simulation (Figure 3(c)), and had significantly lower prediction accuracies. For results of using SSVS, using one neighborhood (fused Lasso) had larger prediction errors and more misdetections on significant model parameters in variable selection (Figure 3(e)). However, increasing the size of neighborhoods enforced in SSVS may significantly improve the modeling results (Figure 3(e) to (i)). When there were more than two neighborhoods considered in variable selection, the prediction error and misdetections in variable selection gradually increased. This simulation did not only show the values of SSVS in spatial variable selection problems, but also emphasize the importance of varying the size of neighborhoods considered for SSVS in order to achieve the best modeling performance.

3.2 A 1-D simulation study of SSVS

Additionally, we created a 1-D data simulation to test the performance of SSVS by varying the sample size of input data (n), the number of model parameters (p), and the covariance of predictors controlled by covariance shrinkage parameter (τ) defined later in this simulation. The sample size had the values of $n = 40$ and $n = 400$, the number of predictors (p) had values of $p = 4000$ and $p = 8000$, and the covariance shrinkage parameter (τ) had values of 1.01 and 1.05. Based on τ, the

covariance between two variables was generated as

$$\sigma_{i+d,i} = \text{cov}(x_{i+d},\ x_i) = \text{cov}(x_{i-d},\ x_i) = \frac{1}{\tau^d},$$

where x_{i-d} and x_{i+d} were the d distances of the variables before and after x_i, respectively. Then, covariance among variables reflects neighborhood shrinkage effects, i.e., the larger the d, the smaller the covariance between x_{i+d} and x_i or x_{i-d} and x_i. Such a neighborhood shrinkage effect was indeed observed in our case study data set when we sort the spatial predictors based on their contrast values from small to large. In total, we had eight simulation scenarios. The model parameters were generated from a uniformly distributed random combination of piece-wise constant functions and exponential decay functions (see Figure 4(a)). If a piece-wise constant function was used, then 100, 150 or 200 parameters in series with equal and non-zero parameter values were generated, and the values were selected from a discrete uniform distribution of {-3, -2, -1, 0, 1, 2, 3}. Similarly, if an exponential decay function was used, 100, 150 or 200 parameters in series were generated using

$$\beta_{i-d} = \beta_{i+d} = \frac{\beta_i}{\theta^d},$$

so that the parameters of each series formed a symmetrical curve that mimicked the shrinkage effect on values of the parameters. Here, β_i was the parameter in the center of each series of parameters and followed a discrete uniform distribution of {-3, -2, -1, 0, 1, 2, 3}. β_{i-d} and β_{i+d} were the d distances of the parameters before or after β_i, respectively, θ was the shrinkage parameter and followed a discrete uniform distribution of {1.01, 1.02, 1.03}, which generated a symmetrically decaying parameter curve. Finally, the response was generated based on model (1) using the values generated above and ε following i.i.d. $N(0, 1)$. The motivation to generate the model parameters containing two different structures was to test if SSVS could better recover the inherent model structure when both piece-wise constant and smooth model parameter structures exist.

Similar to the previous simulation, we used the 90%–10% random data split for training and testing within each replication, with 100 replications performed in total. The tuning parameters were selected based on EBIC. Due to the 1-D nature of the underlying data set, matrix regression was not used for this simulation study. We varied the neighborhood value r from one to five in SSVS (one being fused Lasso) and report only the best result for SSVS with $r > 1$. Table 3 reports average RMSE values for the prediction based on the testing data and the corresponding SE values (shown in parenthesis) over 100 replications for each scenario. We refer to Lasso, where the neighborhood effect was not considered as $r = 0$. The variable selection results are presented in Table 4 based on variable selection accuracies

$$ACC = \frac{True\ Negative + True\ Positve}{Total\ Amount\ of\ Predictors}.$$

The values shown in bold are the best results (smallest errors) obtained under each data generation scenario across different models. The modeling assumptions were validated by residual plots; these are shown in the online supplementary materials. The first observation is that SSVS performed significantly better than did Lasso in all scenarios. Within SSVS models, when the sample size was small ($n = 40$), a larger r offered better prediction accuracy, and when the sample size ($n = 400$) was large, a smaller r offered better prediction accuracy (SSVS with $r = 1$). The results indicate that emphasizing the neighborhood effect of variables can result in a better performance when the sample size is very limited. However, we also realized that when the sample size reduced to only 40, the prediction accuracy of SSVS became much worse, which had approximately 10 times larger
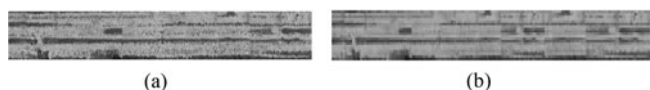
RMSE compared with the "$n = 400$" case. This means that we should always increase the sample size as much as possible for an ideal prediction performance when the model dimension grows very large. Lastly, we can see that SSVS was very robust to the variation on the covariance of adjacent model predictors, compared with Lasso. This suggests that SSVS can effectively handle the data collinearity by considering model parameter smoothness.

As a visual illustration of variable selection, we present the results from the same data set generated with 4000 predictors. Figure 4(a) shows the true parameters generated and Figure 4(b) shows the parameters estimated by SSVS when more than one neighborhood was considered. By comparing the figures, it is clear that when we considered more neighborhoods, SSVS recovered the original parameters significantly better compared with SSVS only considering one neighborhood (Figure 4(c)), and Lasso, which did not consider the neighborhood effect (Figure 4(d)).

4. Case study of the AJP for printed electronics

In this case study, we model the resistance of conducting wires printed by the AJP process. Single-layer silver nanoparticle wires were printed by varying several process parameters, including atomizer power voltage, process speed, gas flow rate, sheath gas flow rate, and ink volume. In the end, 35 wires with microscopic images taken on their surfaces were produced and the corresponding resistances were measured. The primary defect type we are focusing on in this study is missing spray of the silver inks. Such defects can be seen as black pinholes/regions in Figure 5, which significantly increase the resistance of printed wires. A known cause of missing ink spray is the inappropriate compositions of silver nanoparticle inks (Zhao et al., 2012). Some recent research focuses on adding novel carbon nanotubes, which can bridge the pinholes/defects, into silver nanoparticle ink to improve the printing quality (Oh et al., 2008; Zhao et al., 2012). Additionally, other process settings, including the

Figure 5. (a) An original gray-scale image and (b) a newly formed image with lower resolution.
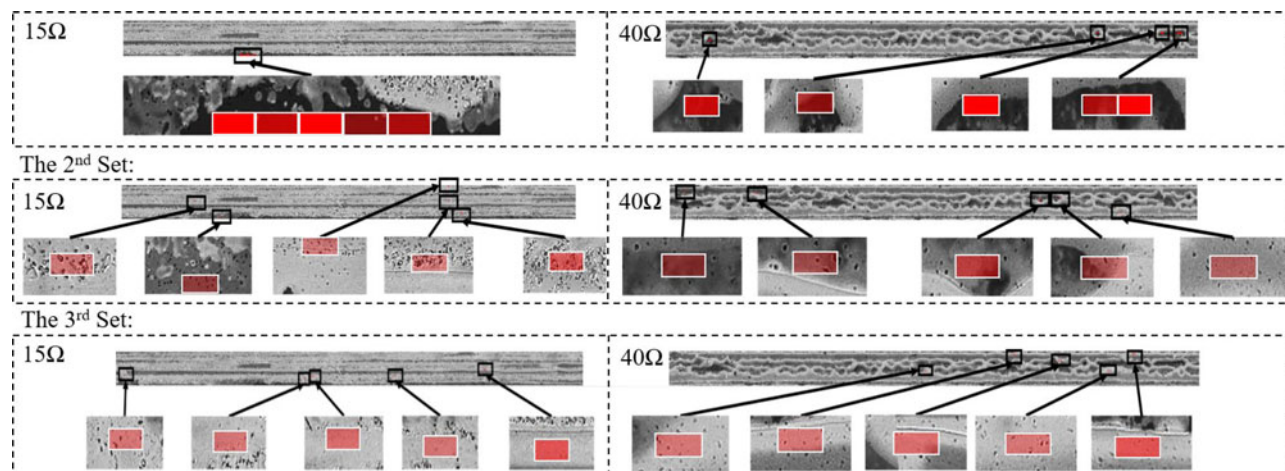
Figure 6. For the first set: the top five selected meshes represent the contrast between each mesh's intensity and the overall image's mean intensity for the wire with 15 Ω and 40 Ω resistances. Second set: the top five selected meshes reflect the contrast between each mesh's intensity and the mean intensity of the each mesh's 8-Connected neighborhood for the wire with 15 Ω and 40 Ω resistances. Third set: the top five selected meshes reflect the contrast between each mesh's intensity and the largest row-wise mean intensity for the wire with 15 Ω and 40 Ω resistances.

Table 5. Testing RMSE values over 100 replications for the AJP data set.

| | Benchmark Models | | | Proposed Model |
	Matrix Regression	SSVS ($r = 0$) / Lasso	SSVS ($r = 1$) / Fused Lasso	SSVS ($r = 3$)
RMSE	8.44 (0.87)	4.68 (0.20)	3.27 (0.14)	**3.21 (0.13)**

sheath gas flow rate, the aerosol gas flow rate, and the stage speed, have been shown to affect the wire resistance and potentially contribute to the missing ink spray issue (Sun et al., 2017).

4.1. Contrast generation on microscopic images

A high-resolution microscopic image (741 × 19491 pixels), combined from 10 consecutive microscopic images, was taken on the conducting wire over a small area (0.5 mm × 10 mm). It can be inefficient and computationally expensive to use one predictor to represent such a small region for product quality characterization. For ease of future modeling scale-up, we divided the raw image (Figure 5(a)) into rectangular meshes and averaged the intensities of all the pixels in each mesh (Figure 5(b)). This approach is also called the average pooling operation with non-overlapping windows (Boureau et al., 2010), and we refer to images produced from the pooling as pooled images. When determining the optimal resolution for images after pooling, we first trained different Lasso models using different sets of pooled images in resolutions of 10 × 100, 20 × 200, 30 × 300, 40 × 400, and 50 × 500 based on the underlying data set as a pilot study. The model trained using the resolution setting of 20 × 200 provided us the best prediction results on the testing data. As a result, each pooled images has a resolution of 20 × 200, with each mesh representing a 50 μm × 25 μm region.

For the case study, we considered three types of contrasts, which could be easily generated from the images without engineering domain knowledge. The first set of 20 × 200 predictors was generated with the contrasts between each mesh's intensity and the overall image's mean intensity. The second set of 20 × 200 predictors was generated with the contrasts between each mesh's intensity and the mean intensity of the meshes in its 8-Connected neighborhood. Lastly, the third set of 20 × 200 predictors was generated with the contrasts between each mesh's intensity and the largest row-wise mean intensity. In an AJP process, this "brightest" region in the microscope image was the outcome of the most silver ink spray and could be considered as the most conductive path of the wire. However, one problem is that defect locations can vary significantly from one wire to another (dark regions in Figure 6), so that it was meaningless to fix each predictor to one corresponding location of images. Therefore, we sorted the values within each set of predictors from low to high and re-organized the predictors in quantiles. As a result, we expected that predictors at certain quantiles (e.g., high quantiles representing high contrast regions) were more strongly associated with wire resistance. Furthermore, the neighborhood effect among the model parameters of neighborhood quantiles is preserved, which

means that the changes of parameter values among neighborhood quantiles should be smooth. As a result, we can apply the 1-D version of the SSVS model based on spatial predictors sorted in quantiles.

We adopted High-dimensional Ordinary Least squares Projection (HOLP) by Wang and Leng (2015) to further filter the 12000 (3×20×200) predictors down to 6000 predictors. Here, the HOLP method is a screening method, which is built on the Ordinary Least Square (OLS) estimator. Comparing with regularized regressions, HOLP can quickly screen the number variables in the original variable space down to a relatively low level, so that the computational efficiency of SSVS can be further enhanced. We consider that determining the appropriate percentage of variables to preserve through HOLP can be a valuable future study. One thing worth emphasizing on dimension reduction in this work is that there are other popular methods, such as Principal Component Analysis (PCA) (Jin and Shi, 2000), to reduce the dimension of the data. However, different from HOLP, methods like PCA are widely known as "black box" approaches, which do not preserve the original variables of data, and hence are significantly detrimental to the interpretability of the modeling and variable selection efforts.

4.2. Numerical results and interpretations

We performed 100 replications for both benchmarks (Lasso and nuclear-norm-based matrix regression) and SSVS estimator under different neighborhood settings. For fair comparison, the matrix regression, which already incorporated low-rank regularization in model estimation, was trained using the original 2-D microscopic image data (Zhou and Li, 2014), whereas the SSVS and Lasso were trained using the proposed spatial predictors in 1-D filtered quantiles.

For each replication, we used 90%–10% data partition for model training and testing. The average testing RMSE values for the resistance obtained over 100 replications are presented in Table 5 with SE values in the parenthesis. The regularized matrix regression has a significantly poorer prediction performance compared with the proposed approach. As a drawback mentioned previously, one major limitation on regularized matrix regression is that it fixes each predictor to the same location across different samples, but the defect areas which are strongly associated with the response (resistance) are constantly changing their locations. Furthermore, we can see that Lasso performed poorly in resistance prediction. On the contrary, SSVS with different neighborhood settings had significantly smaller RMSE values, and the smallest error was achieved at $r = 3$. This indicated that the neighborhood defined by $r = 3$ was the most appropriate to describe the predictors' smoothness. The

modeling assumptions were validated by residual plots that are available in the online supplementary materials.

One of the advantages of transforming original images directly into spatial predictors lies in good interpretability, as complicated feature extractions can lead to the loss of information depending on how well the underlying physical manufacturing process is understood. We illustrate the most selected features in Figure 6, where the colors of the mask indicate the number of times a predictor was selected over 100 replications (a darker color indicates the mesh being more frequently selected). Specifically, the top two wires of Figure 6 illustrate the variable selection among the first set predictors: the contrasts between each mesh's intensity and the overall image's mean intensity. The middle two wires of Figure 6 illustrate the variable selection among the second set predictors: the contrasts between each mesh's intensity and the mean intensity of the mesh's 8-Connected neighborhood. The bottom two wires of Figure 6 illustrate the variable selection among the third set predictors: contrasts between each mesh's intensity and the largest row-wise mean intensity of the image. The row with the largest intensity, due to a dense layer of ink sprayed, is the most conductive path of the wire.

For the first set in Figure 6, the selected meshes identified the missing ink defects. However, the intensities of selected meshes in the 40 Ω-wire were only 78 units (on a 0–255 scale) darker than the wire mean intensity on average, with the difference increasing to 120 units for the 15 Ω-wire. A relatively lower difference is due to the mean intensity of the 40 Ω-wire being low, which is the result of excessive missing prints shown in the image. For the second set in Figure 6, the selected meshes identified the areas of non-uniform ink spray (seen as black pinholes). However, the contrasts between each mesh and its 8-Connected neighborhood were significantly smaller for the 15 Ω-wire, which is on average 0 versus -4 for the 40 Ω-wire. The lower contrast reflects that the 15 Ω-wire was printed more uniformly. For the third set in Figure 6, the selected meshes identified uniformly printed regions. The meshes in the 15 Ω-wire have similar intensity to that of the image's largest row-wise mean intensity (an average difference of zero). On the contrary, the meshes for the 40 Ω-wire are on average 9 units darker than its largest row-wise mean intensity due to significantly more missing sprays. The variable selection results show that variation modeling based on simple and direct spatial features have inherently good interpretability for quality diagnosis and can result in an accurate resistance prediction when combined with SSVS estimator.

5. Summary

Although spatial predictors are widely encountered in AM process modeling, the modeling and feature extractions of the spatial predictors are typically challenging and case-specific problms. In most cases, such an effort requires engineering knowledge of the spatial data set (e.g., feature extractions from images), or the manufacturing process. In this article, the proposed SSVS aims to identify the significant predictors in pursuit of smooth parameters to reflect the neighborhood effect. The size of neighborhoods can be adaptively determined by the data set, which is flexible for various AM processes, with different spatial correlations of predictors. The proposed SSVS relaxed the strong assumption of fused Lasso, which is SSVS's special case considering a 1-neighborhood, and was able to estimate the underlying model parameters with higher accuracy. Both the simulation and case studies showed that the proposed methodology could not only accurately predict the quality response, but also automatically locate areas in quality modeling, which can be used in root cause diagnosis.

There are several directions for further investigations. First, we can validate the proposed methodology on other types of 2-D or 3-D spatial data sets, which have coherent spatial information across different samples, so that re-organizing the spatial data into quantiles for smoothness enforcement is no longer necessary. Second, we may also relax the coherency requirement by projecting the raw image data into other domains, e.g., 2-D Fourier domains, so that the same set of projected spatial predictors may correspond to different regions with missing spray defects across different samples. As a result, ordering the predictors in quantiles will no longer be necessary before adopting SSVS for the AJP case study data set. Third, we may adopt other spatial data sets to enhance the modeling performance. For example, we can use 3-D surface scanning to capture the thickness variation, which can also contribute to the resistance variation of printed wires. However, limitations, such as a slow data collection speed, of the current sensing technologies suggest that additional spatial data types might not be obtained efficiently for quick product quality quantification (Wang et al., 2013). Finally, the proposed framework can be further used for spatial predictor monitoring and control for quality improvements and variation reduction, with some examples in Li, Mohan, Sun, and Jin (2017). The code package of SSVS is available upon request.

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