Spatial Randomness-Based Anomaly Detection Approach for Monitoring Local Variations in Multimode Surface Topography

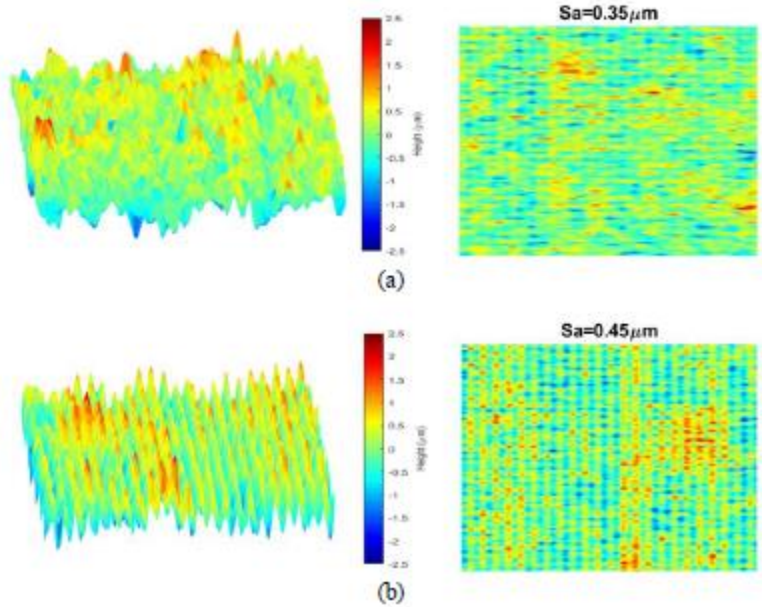
한양대학교 산업공학과
IDSL 석사과정 고경준

Contents

1. Intordaction

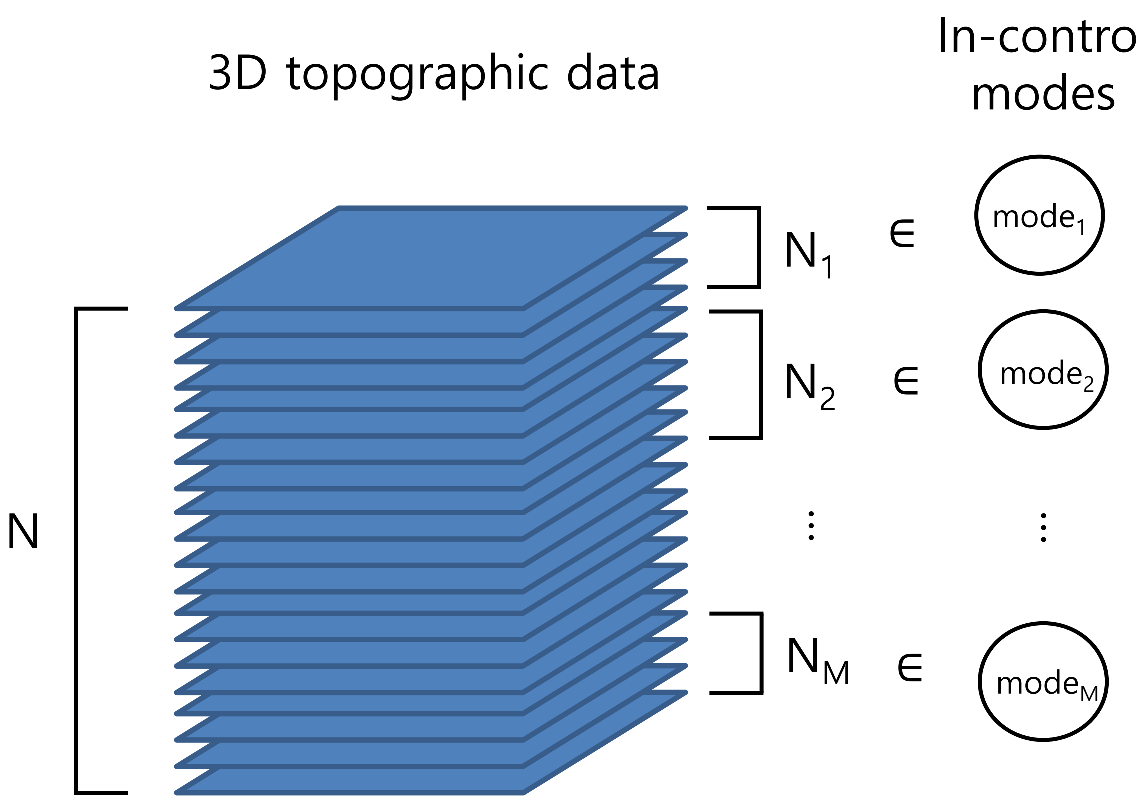
Anomaly detection of 3D topographic data

- 부자재 surface topography 상태는 완제품의 상태 및 성능에 큰 영향을 끼침
- 특히 종이 산업에서는 surface topography가 제품의 품질 자체
- 3D topographic data monitoring에서 spatial autocorrelation 문제를 고려해야 함
- Complex manufacturing procedures에서는 대부분 multi-mode in-control topographic



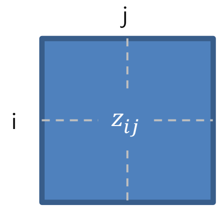
2. Spatial Randomness-Based Anomaly Detection

2.0 data description



2. Spatial Randomness-Based Anomaly Detection

2.1 Multimode Surface Binarization



- **Surface topographic data Z =** $[z_{ij}]$ **라고 할 때, (**z_{ij} = height value**)**
  single mode prediction model은 (1)과 같음.

$$z_{ij} = f(\mathbf{y}_{ij}) + \varepsilon_{ij}, \qquad \varepsilon_{ij} \sim iid\ N(0,\ \sigma^{m}) \tag{1}$$

* y_{ij} = set of adjacent height values, $f(\cdot)$ = appropriate regression model with $\{y_{ij},\ z_{ij}\}$

- **Multi mode prediction model은 (2)와 같음.**

$$z_{ij}^{(m)} = f_m(\mathbf{y}_{ij}^{(m)}) + \varepsilon_{ij}^{(m)}, \qquad \varepsilon_{ij}^{(m)} \sim iid\ N(0,\ \sigma_m^2) \tag{2}$$

- **이 때,** $y_{ij}^{(m)}$**는** $z_{ij}^{(m)}$**의 neighboring height values 중 spatial distance** l_m **내에 있는 값**
- **Cross-validated R^2를 이용해 optimal** l_m**를 결정**

2. Spatial Randomness-Based Anomaly Detection

2.1 Multimode Surface Binarization

- Residual matrix $R^{(m)}$ = $[r_{ij}^{(m)}]$은 (3)과 같음.

$$r_{ij}^{(m)} = z_{ij} - f_m(\mathbf{y}_{ij}^{(m)}) \tag{3}$$

- Residual의 pattern을 통해 mode를 구분하고 topographic variations를 확인할 수 있음
- 하지만 residual patterns는 defective area의 크기가 작으면 파악하기 어려움

→ local change description 향상을 위해 mode-specific binary representation 제안.

- Binarized surface matrix $B^{(m)}$ = $[b_{ij}^{(m)}]$는 (4)과 같음.

$$\mathbf{B}^{(m)} = [b_{ij}^{(m)}],\ b_{ij}^{(m)} = \begin{cases} 1, & \left|r_{ij}^{(m)}\right| \geq T^{(m)} \\ 0, & \text{otherwise} \end{cases} \tag{4}$$

- 이 때 $b_{ij}^{(m)}$ = 1인 경우 'suspicious residual'로 표현

2. Spatial Randomness-Based Anomaly Detection

2.2 Comparing Spatial Randomness Based on Kullback-Leibler Divergence

- 만약 B안의 suspicious residuals가 spatially randomly distributed 되었다면 complete spatial randomness(CSR)라고 함
- CRS인 경우 suspicious residual는 Poisson point process를 따른다고 가정
- D_k= B에서 무작위로 선택된 suspicious residual과 K개의 NN과의 거리를 나타내는 rv

- D_k의 cumulative probability는 (5)와 같음

$$F_{D_K}(d) = P(D_K \le d) = 1 - \sum_{k=0}^{K-1} P\left(N[C_d(s)] = k \mid \lambda_K\right) = 1 - \sum_{k=0}^{K-1} \frac{\left(\pi \lambda_K d^2\right)^k}{k!} e^{-\lambda_K \pi d^2} \qquad (5)$$

$C_d(s)$ = circular area with radius ‘d’ around ‘s’. (s = coordinate of suspicious residual)

$N[C_d(s)]$ = the total number of suspicious residuals in $C_d(s)$

λ_K = expected density of suspicious residuals

(Cressie, 2015)

2. Spatial Randomness-Based Anomaly Detection

2.2 Comparing Spatial Randomness Based on Kullback-Leibler Divergence

$$f(x; a, d, p) = \frac{(p/a^d)x^{d-1}e^{-(x/a)^p}}{\Gamma(d/p)}$$

- Density f_{D_k}는 F_{D_k}의 미분으로 (6)처럼 계산

$$f_{D_K}(d) = F'_{D_K}(d) = \frac{e^{-\lambda_K \pi d^2} 2(\pi\lambda_K)^K d^{2K-1}}{(K-1)!}. \qquad (6)$$

- $D_k \sim GG(\frac{1}{\sqrt{\lambda_K \pi}}, 2K, 2)$. (Generalized Gamma distribution)

- B_1, B_2를 비교하기 위해 KL Divergence idea를 활용. $KL(f_1 | f_2)$

$$D_{KL}(f_1, f_2) = \mathrm{E}_{f_1}\left[\log\frac{f_1(x)}{f_2(x)}\right] = \int f_1(x)\left(\log f_1(x) - \log f_2(x)\right)dx \qquad (8)$$

2. Spatial Randomness-Based Anomaly Detection

2.2 Comparing Spatial Randomness Based on Kullback-Leibler Divergence

- spatial randomness Kullback-Leibler(SRKL) divergence를 제시

$$D_{SRKL}(\mathbf{B}_1,\mathbf{B}_2)=\mathrm{E}_{f_{D_{K,1}}}\left[\log\frac{f_{D_{K,1}}\left(x \mid 1/\sqrt{\lambda_{K,1}\pi},2K,2\right)}{f_{D_{K,2}}\left(x \mid 1/\sqrt{\lambda_{K,2}\pi},2K,2\right)}\right] \quad (9)$$

$$D_{SRKLS}(\mathbf{B}_1,\mathbf{B}_2)=D_{SRKL}(\mathbf{B}_1,\mathbf{B}_2)+D_{SRKL}(\mathbf{B}_2,\mathbf{B}_1). \quad (10)$$

$$\begin{aligned}D_{SRKLS}(\mathbf{B}_1,\mathbf{B}_2)&=\left(\frac{KT_1/\pi\sum_{t_1=1}^{T_1}d_{t_1}^2}{KT_2/\pi\sum_{t_2=1}^{T_2}d_{t_2}^2}\right)^K+\left(\frac{KT_2/\pi\sum_{t_2=1}^{T_2}d_{t_2}^2}{KT_1/\pi\sum_{t_1=1}^{T_1}d_{t_1}^2}\right)^K-2K\\&=K\left\{\left(\frac{T_1\sum_{t_2=1}^{T_2}d_{n_{S_2}}^2}{T_2\sum_{t_1=1}^{T_1}d_{t_1}^2}\right)^K+\left(\frac{T_2\sum_{t_1=1}^{T_1}d_{t_1}^2}{T_1\sum_{t_2=1}^{T_2}d_{t_2}^2}\right)^K\right\}-2K.\end{aligned} \quad (11)$$

- (11) is Closed form of (10)
- B_1, B_2의 spatial pattens가 같을 경우 $T_1\sum_{t_2=1}^{T_2}d_{t_2}^2=T_2\sum_{t_1=1}^{T_1}d_{t_1}^2$

2. Spatial Randomness-Based Anomaly Detection

2.3 Identifying the Variations in Surface Topography

- Historical surface data $\mathbf{D}_{IC}^{(m)} = \{\mathbf{Z}_1^{(m)}, \ldots, \mathbf{Z}_n^{(m)} \ldots, \mathbf{Z}_{N_m}^{(m)}\}$
- Binary representation $\mathbf{L}_{IC}^{(m)} = \{\mathbf{B}_1^{(m)}, \ldots, \mathbf{B}_{N_m}^{(m)}\}$
- new data Z_{new} , $B_{new}^{(m)}$
- 위 상황에 대해 average SRKLS를 계산하여 최적 mode 파악 및 anomaly detection

$$S_{SRKL} = \min_m \left\{ \frac{1}{N_m} \sum_{n=1}^{N_m} D_{SRKLS}\left(\mathbf{B}_{new}^{(m)}, \mathbf{B}_n^{(m)}\right) \right\}. \quad (12)$$

$$m^* = \arg\min_m \left\{ \frac{1}{N_m} \sum_{n=1}^{N_m} D_{SRKLS}\left(\mathbf{B}_{new}^{(m)}, \mathbf{B}_n^{(m)}\right) \right\}. \quad (13)$$

- 기준값과 비교하여 abnormal 여부 판단 $S_{SRKL} > U^{(m^*)}$

3. Simulation Study

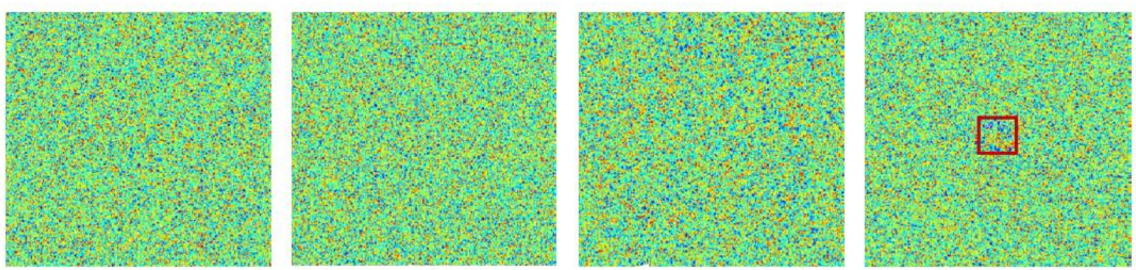
3.1 Simulation Setup

- **Normal surface data with size 250×250를 (14)번 식에 따라 생성**

$$z_{ij} = \phi_1 z_{i-1j} + \phi_2 z_{ij-1} + \varepsilon_{ij} \text{ where } \varepsilon_{ij} \sim iid\, N(0, \sigma^2). \qquad (14)$$

- **3가지 모드를 ϕ_1, ϕ_2 = (0.13, 0.01), (0.01, 0.13), (0.20, 0.19), σ^2는 동일하게 가정**
- **Local defect는 2%, 5%, 8%의 size로 3가지 종류 생성**

  ϕ_1, ϕ_2 = (0.40, 0.40), (0.43, 0.43), (0.46, 0.46), σ^2는 동일하게 가정



(a) Mode 1 (b) Mode 2 (c) Mode 3 (d) Abnormal surface

3. Simulation Study

3.2 Performance Comparison

- 300개의 normal, abnormal surfaces 생성. (각 모드별 100개씩)
- Classification accuracy(17)와 Overall accuracy(18)를 비교

$$\textit{Classification accuracy} = \mathrm{E}\left(\frac{\sum_{m=1}^{M} I_m + I_A}{\sum_{m=1}^{M} N_m + N_A}\right) \tag{17}$$

$$\textit{Overall accuracy} = \mathrm{E}\left(\frac{I_N + I_A}{\sum_{m=1}^{M} N_m + N_A}\right) \tag{18}$$

- I_m = true identification of normal under m^{th} in-control mode
- I_A = true identification of abnormal under m^{th} in-control mode
- N_m = total number of normal under m^{th} in-control mode
- N_A = total number of abnormal under m^{th} in-control mode

3. Simulation Study

3.2 Performance Comparison

- **Comparison of the overall accuracy with single/multi mode AD models**

Variation type	Size of defect (Söderfjäll et al.)	Surface monitoring approaches							
		Single mode approaches					Multimode approaches		
		S_a	S_{ds}	S_W	S_{PSD}	S_{AD}	S_{MAD}	S_{MF}	S_{SRKL}
Mild variation ($\phi_1 = 0.40$, $\phi_2 = 0.40$)	2	0.537	0.507	0.520	0.562	0.515	0.533	0.509	**0.604**
	5	0.613	0.547	0.568	0.621	0.604	0.697	0.538	**0.830**
	8	0.620	0.587	0.619	0.623	0.763	0.836	0.559	**0.909**
Moderate variation ($\phi_1 = 0.43$, $\phi_2 = 0.43$)	2	0.568	0.512	0.530	0.597	0.544	0.580	0.530	**0.719**
	5	0.622	0.563	0.597	0.624	0.748	0.824	0.573	**0.926**
	8	0.622	0.611	0.635	0.637	0.930	0.909	0.598	**0.966**
Severe variation ($\phi_1 = 0.46$, $\phi_2 = 0.46$)	2	0.607	0.523	0.545	0.620	0.628	0.694	0.577	**0.875**
	5	0.626	0.589	0.625	0.669	0.937	0.930	0.651	**0.967**
	8	0.780	0.631	0.644	0.948	0.968	0.962	0.694	**0.969**

3. Simulation Study

3.2 Performance Comparison

- **Comparison of the classification accuracy with multi mode AD models**

Variation type	Size of defect	Multimode approaches		
		S_{MAD}	S_{MF}	S_{SRKL}
Mild variation ($\phi_1 = 0.40$, $\phi_2 = 0.40$)	2	0.533	0.250	**0.602**
	5	0.697	0.273	**0.828**
	8	0.837	0.296	**0.907**
Moderate variation ($\phi_1 = 0.43$, $\phi_2 = 0.43$)	2	0.580	0.271	**0.715**
	5	0.824	0.304	**0.924**
	8	0.908	0.336	**0.963**
Severe variation ($\phi_1 = 0.46$, $\phi_2 = 0.46$)	2	0.694	0.313	**0.873**
	5	0.930	0.383	**0.963**
	8	0.962	0.436	**0.967**

3. Simulation Study

3.3 Selection of the Parameter K

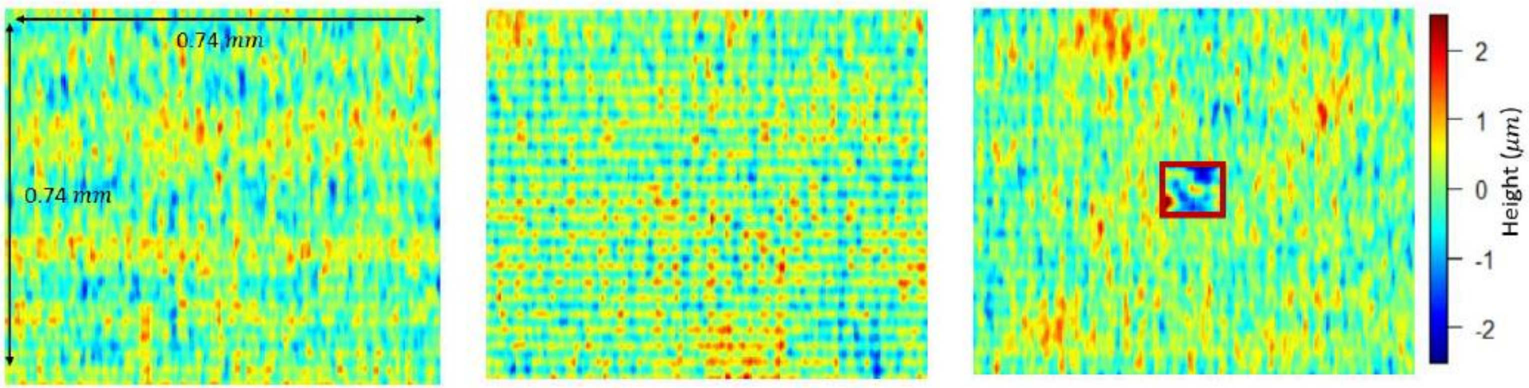
- K = Suspicious residual과 비교될 주변 점의 개수 (KNN)

Variation type	Size of defect	Values of k			
		$K=1$	$K=5$	$K=10$	$K=15$
Mild variation ($\phi_1 = 0.40$, $\phi_2 = 0.40$)	2	0.565	0.598	0.605	0.605
	5	0.645	0.738	0.738	0.713
	8	0.795	0.868	0.877	0.863
Moderate variation ($\phi_1 = 0.44$, $\phi_2 = 0.44$)	2	0.768	0.807	0.825	0.810
	5	0.873	0.913	0.930	0.923
	8	0.965	0.977	0.970	0.965
Severe variation ($\phi_1 = 0.48$, $\phi_2 = 0.48$)	2	0.867	0.888	0.902	0.898
	5	0.953	0.960	0.965	0.960
	8	0.977	0.977	0.970	0.965
Average overall accuracy		0.823	0.858	**0.865**	0.856

4. Case Study : in Paper Surface

4.1 Multimode Surface Topography in Paper Surface

- Paper industry에서는 surface status가 매우 중요한 issue
- Multi mode가 존재한다.



(a) (b) (c)

4. Case Study : in Paper Surface

4.2 Monitoring Local Variations in Paper Surface

- Normal surface data with size 200×200
- Normal and abnormal 각 20개씩 실험

Size of defect	Surface monitoring approaches							
	Single mode approaches					Multimode approaches		
	S_a	S_{ds}	S_W	S_{PSD}	S_{AD}	S_{MAD}	S_{MF}	S_{SRKL}
2	0.600	0.500	0.500	0.675	0.575	0.600	0.600	**0.700**
5	0.725	0.500	0.475	0.925	0.725	0.750	0.675	**0.950**
8	0.925	0.500	0.525	0.925	0.850	0.875	0.750	**0.975**

Size of defect	Multimode approaches		
	S_{MAD}	S_{MF}	S_{SRKL}
2	0.600	0.375	**0.700**
5	0.750	0.450	**0.950**
8	0.875	0.525	**0.975**

5. Conclusions

Contributions

- Multimode surface binarization model를 제안하여 작은 defect도 파악 가능
- Spatial randomness KL divergence 방법 제안하여 surfaces를 비교 가능
- Simulation 및 실제 데이터에서 좋은 성능을 보이는 AD model 제안

Further study

- Defective regions의 root cause를 파악하는 모델 개발
- 더 복잡한(multi features) 3D topographic data에 활용가능한 모델 개발

감사합니다.