Profile Control Charts

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at
Fall Technical Conference
Indianapolis, IN
08 October, 2009

Thanks to my Collaborators

Wei, Ying (Columbia Univ)
Zhao, Zhibiao (Penn State)
Zhu, Junjia (Penn State)

Time Series101: Univariate Time Series

135, 143, 127, 129, ..., 172 What's next?

$y_1, y_2, \ldots, y_T$ What's $\hat{y}_{T+1}$?

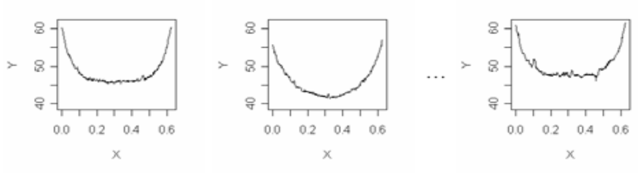
Model Building and Forecasting (short/long term)
Monitoring (Quality Assurance)
Change Point Problem

Time Series201: Multivariate Time Series

$\begin{pmatrix} 5 \\ 143 \\ 85 \\ 46 \end{pmatrix}, \begin{pmatrix} 12 \\ 174 \\ 77 \\ 39 \end{pmatrix}, \ldots, \begin{pmatrix} 16 \\ 191 \\ 81 \\ 41 \end{pmatrix}$ What's next?

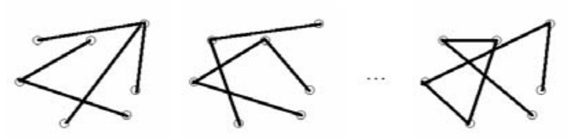
$\vec{y}_1, \vec{y}_2, \ldots, \vec{y}_T$ What's $\hat{\vec{y}}_{T+1}$?

Time Series301: Functional Data (Profile)



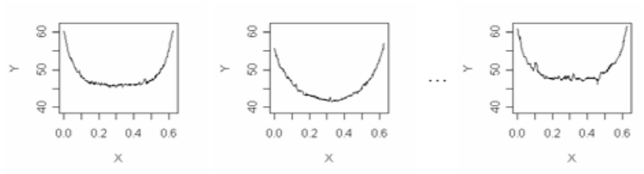
$f_1, f_2, \ldots, f_T$ What's $\hat{f}_{T+1}$?

Time Series 401: Graphic/Network
(Link Prediction, Communication Network)



$G_1, G_2, \ldots, G_T$ What's $\hat{G}_{T+1}$?

Today's Talk is about
Monitoring Functional Data (Profile)



In general, there are more than on X.

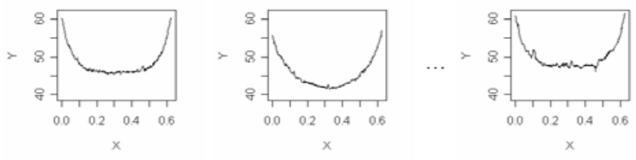
Process Monitoring

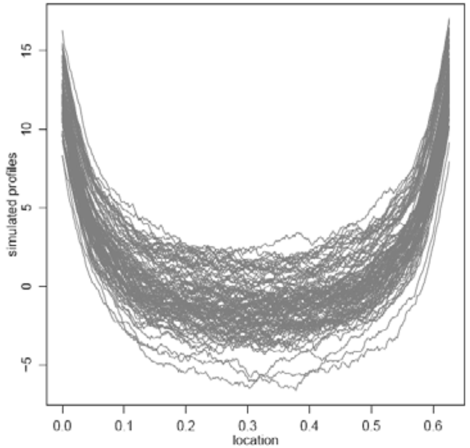
- Phase-I
  - Understand the variation in a process over time.
  - Evaluate the process stability
  - Model the in-control process performance
  - Evaluated by Probability of Signal (POS)
- Phase-II
  - Monitoring the process, using on-line data
  - Evaluated by Run-Length Distribution (ARL)

Example 1: (Full) VDP Data

- Vertical Density Profile (VDP)
  - The density fiber-board which determines its machinability
  - *Walker and Wright (2002)*
- *Y=the density of the wood board*
  - Measured by using a profilometer
  - Uses a laser device to take measurements
- *X=the depth of thickness of the board*

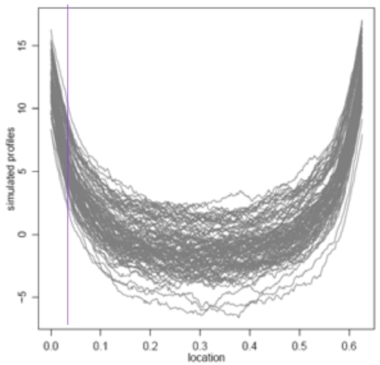
Monitoring Functional Data (Profile)





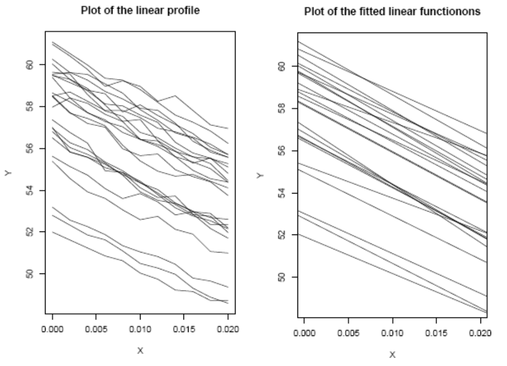
Example 2: truncated VDP Data (Edge)

For vertical density close to the wood surface —only the density close to the top is relevant



Truncated VDP Data

for vertical density close to the wood surface—only the density close to the top is relevant ($x \le 0.02$)



Intercept:
Surface density in each wood board

Slope:
the speed of density increase as depth goes

Truncated VDP Data

Investigation on the speed of density increase as depth goes (ie, Slope)

Naïve Approach: Simple Linear Model

Model:

$$y_{ji} = A_0 + A_1 x_{ij} + \varepsilon_{ij} \qquad \varepsilon_{ij} \sim N(o, \sigma^2)$$

$$LCL = A_1 - z_{\alpha/2} * \sqrt{\frac{\sigma^2}{S_{xx}}}$$

$$UCL = A_1 + z_{\alpha/2} * \sqrt{\frac{\sigma^2}{S_{xx}}}$$

Proposed Method (Zhu and Lin, QE)

Step 1 Check assumptions for each profile: (1) linearity assumption between x and Y; and (2) normality and independence assumption for the residuals.
If any of these assumptions is violated, the corresponding profile may be removed from the dataset. We denote the number of remaining profiles after step 1 as k.

Step 2 Center both x and Y, and estimate the values of parameters: with $\hat{A}_1 = \frac{\sum_{j=1}^{k} a_{1j}}{k}$ and $\hat{\sigma}^2 = \frac{\sum_{j=1}^{k} MSE_j}{k}$.

Step 3 Build the control chart for monitoring the slopes, with the centerline equals to $\hat{A}_1$. $LCL = \hat{A}_1 - t_{k(n-2),\alpha/2} * \hat{\sigma}\sqrt{\frac{k-1}{kS_{xx}}}$, and $UCL = \hat{A}_1 + t_{k(n-2),\alpha/2} * \hat{\sigma}\sqrt{\frac{k-1}{kS_{xx}}}$, where $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2$ and $t_{k(n-2),\alpha/2}$ is the $100(1-\alpha/2)$th percentile of the student t distribution with $k(n-2)$ degrees of freedom.

Step 4 Any profile whose estimated slope falls outside the control limits is regarded as an outlier.

- If no outlier is detected then one concludes that the process is stable and moves to the next step.
- If at least one outlier is detected, then one removes the profile with the largest deviance of slope from the centerline, i.e. remove the profile j with *maximum* $|a_{1j} - \hat{A}_1|$ value. And repeat step 2 and step 3 on the remaining profile dataset until no outliers are detected.

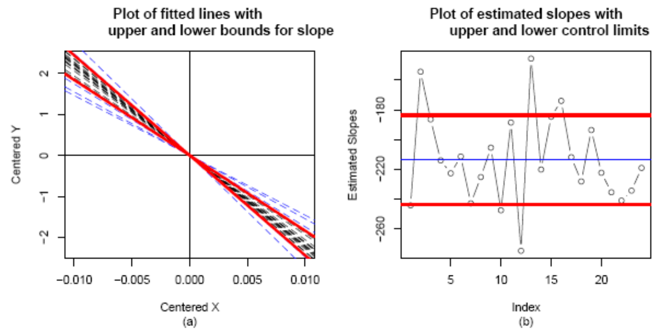
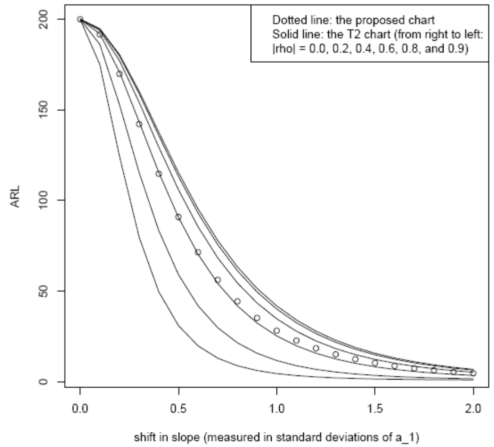


Figure 3: Control Chart for Slopes: Based on the Truncated VDP Data

ARL Comparison with T^2-Chart



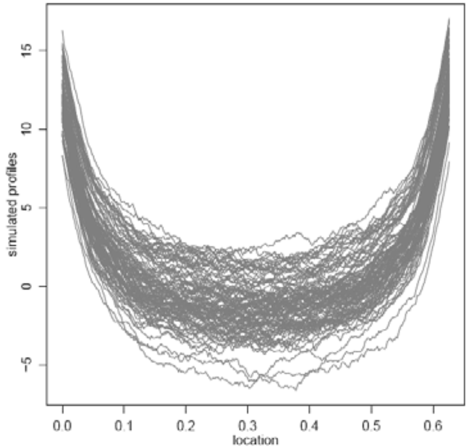
Monitoring the Slope of Linear Profiles

Zhu, J.J. and Lin, Dennis K.J.

Quality Engineering

forthcoming

Now, return to the full VDP data



Model Setting

$$Y_{i,j} = \xi_i + \mu(x_{i,j}) + s(x_{i,j})e_{i,j},$$

$$1 \le j \le m_i, 1 \le i \le n$$

- median$(e_{i,j}) = 0$ and median$(|e_{i,j}|) = 1$.
- $\xi_i =$ median$(Y_{i,j})_{j=1,\ldots,m_i}$, which represents the vertical location of the ith profile
- $\mu(x)$ is the conditional median function of $Y - \xi_i$ given $X = x$. It represents the standard shape of a normative centered response profile. We hence call it *reference profile function*.
- $s(x)$ is essentially the conditional Median Absolute Deviance(MAD) of $Y - \xi$ given $X = x$. We call $s(x)$ the *reference deviation function*, which measures to what extend a normative profile could deviate from the reference profile at a given location x.

Why L-1 Regression?

- **Ordinary least squares (L-2) regression:** the effect of predictors on the mean of Y

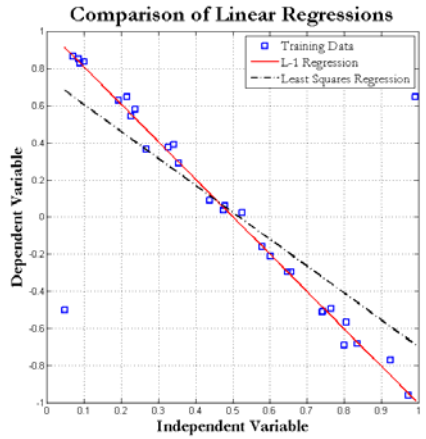
$$\widehat{\beta} = \arg\min \sum_{i=1}^{n} (y_i - x_i^\top \beta)^2$$

- **Median (L-1) regression:** the effect of predictors on the median of Y

$$\widehat{\beta} = \arg\min \sum_{i=1}^{n} |y_i - x_i^\top \beta|$$

  - Root-n consistency
  - Asymptotically normally distributed
  - Invariant to monotone transformation of Y
  - Robust. The estimators are much less sensitive to the outliers, comparing to the least square regression.

L-1 Regression (Robustness)



Estimation of $\mu(x)$

- Initial estimate of $\mu(x)$

$$\hat{\mu}_{b_n}(x) = \arg\min_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{m_i} |Y_{i,j} - \theta| K_{b_n}(x_{i,j} - x).$$

- a bias-corrected jackknife estimator

$$\tilde{\mu}_{b_n}(x) = 2\hat{\mu}_{b_n}(x) - \hat{\mu}_{\sqrt{2}b_n}(x)$$

  to remove the bias in $\hat{\mu}_{b_n}(x)$;
- we show that $\tilde{\mu}_{b_n}$ is uniformly consistent, and asymptotically normally distributed for any x.

Estimation of $s(x)$

- Following the estimate of $\mu(x)$, we have initial estimate $s(x)$

$$\hat{s}_{h_n}(x) = \arg\min_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{m_i} \Big| |Y_{i,j} - \tilde{\mu}_{b_n}(x)| - \theta \Big| K_{h_n}(x_{i,j} - x)$$

- an bias-corrected jackknife estimator of $s(x)$, i.e.

$$\tilde{s}_{h_n}(x) = 2\hat{s}_{h_n}(x) - \hat{s}_{\sqrt{2}h_n}(x).$$

- we also show that $\tilde{s}_{h_n}(x)$ is uniformly consistent, and enjoys asymptotic normality.

Modeling the Profile Curves

Let $(x_{i,j}, O_{i,j})$ be Phase I data consists of n profiles.

1. Define the center of the profile as $\xi_i = \text{median}(O_{i,j})_{j=1,..,m_i}$, which represents the vertical location of the ith profile
2. Present the *centered* profiles, $Y_{i,j} = O_{i,j} - \xi_i$, with the proposed nonparametric location-scale model,

$$Y_{i,j} = \mu(x_{i,j}) + s(x_{i,j})e_{i,j}, \quad 1 \leq j \leq m_i, 1 \leq i \leq n. \tag{6}$$

- $\mu(x)$ as *reference profile*, representing the standard shape of a normative centered response profile
- $s(x)$ as *reference deviation*, which measures to what extend a normative profile could deviate from the reference profile at a given location x.

Key issues to be monitored

1. First, there might be a vertical shift, i.e., the profile may be unusually higher or lower than the normative ones.

   $\Rightarrow$ monitor the center of profiles, i.e. ξ_i's
2. Second, the shape of the new profile may different from the normative ones.

   $\Rightarrow$ Two deviation scores to monitor the shape of the profiles

Measure for Vertical Deviation

- Standardize individual profile centers:

$$d_i = |\xi_i - \mu_\xi| / s_\xi$$

— μ_ξ as the median of ξ_i's, the centers of phase I profiles,

— s_ξ as the median absolute deviation of ξ_i's

- d_i's provide a ranking of the phase I profiles from inside to the outside.
- **the screening threshold**: $(1-\alpha)$th upper quantile of the reference distribution(empirical distribution of $d_i' s$)

Measures for Shape Deviation (1/2)

1. Centering removes the systemic distances among the profiles. Consequently, the main differences between a new centered profile Y_j and the reference curve $\mu(x)$ are mainly due to their different profile shapes.
2. Screening shape deviation based on standardized residuals

$$\hat{e}_j := \frac{Y_j - \tilde{\mu}_{b_n}(x_j)}{\tilde{s}_{h_n}(x_j)}, \quad 1 \leq j \leq m, \quad ($$

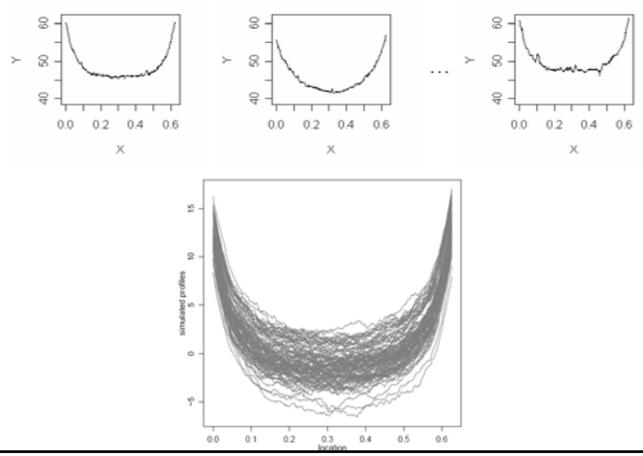
Measures for Shape Deviation (2/2)

$$\hat{e}_j := \frac{Y_j - \tilde{\mu}_{b_n}(x_j)}{\tilde{s}_{h_n}(x_j)}$$

$$T_m^{(1)} = \max_{1 \le j \le m} |\hat{e}_j|, \quad \text{and} \quad T_m^{(2)}(\lambda) = \sum_{j=1}^{m} |\hat{e}_j|^{\lambda}, \quad \lambda > 0.$$

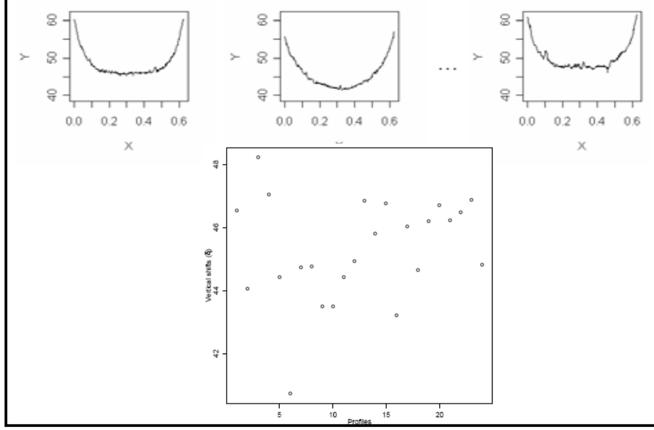
- The first statistic $T_m^{(1)}$ measures the maximal local shape deviation of the new profile from the reference profile;
- while the second score $T_m^{(2)}(\lambda)$ measures its cumulative overall shape deviation from the reference profile.
- The two scores compensate each other, and provide a comprehensive monitoring of shapes.

The VDP data



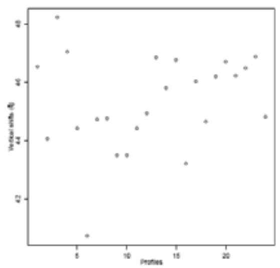
Median Vertical Densities *for each profile*

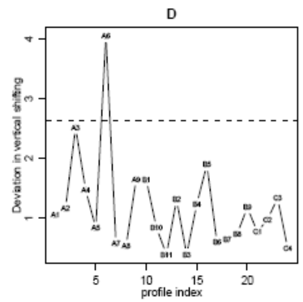
(median is known to be more robust than mean)



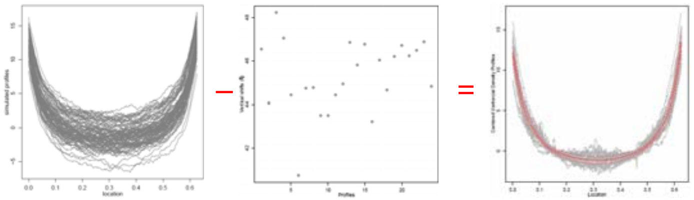
a. Relative Vertical Deviation

$$d_i = |\xi_i - \mu_\xi| / s_\xi$$

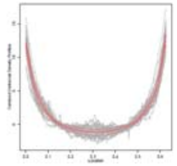




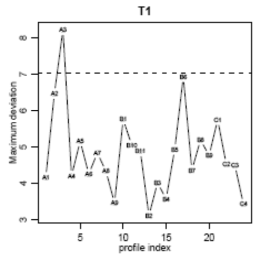
b. Centered (by median) VDP Profiles

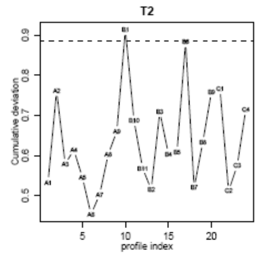


Post-centering deviations



$$T_m^{(1)} = \max_{1 \le j \le m} |\hat{e}_j| \qquad T_m^{(2)}(\lambda) = \sum_{j=1}^{m} |\hat{e}_j|^{\lambda}$$





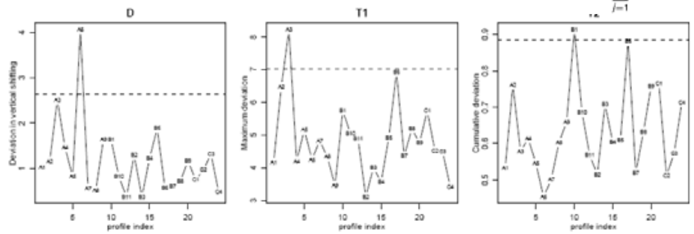
Choices of α

$$\alpha^* = \max_{\alpha} \left\{ \alpha : \sum_{i=1}^{n} \max\{\mathbf{1}_{\{d_i > c^{(0)}(\alpha)\}}, \mathbf{1}_{\{t_i^{(1)} > c^{(1)}(\alpha)\}}, \mathbf{1}_{\{t_i^{(2)} > c^{(2)}(\alpha)\}}\} < n\alpha_0 \right\}$$

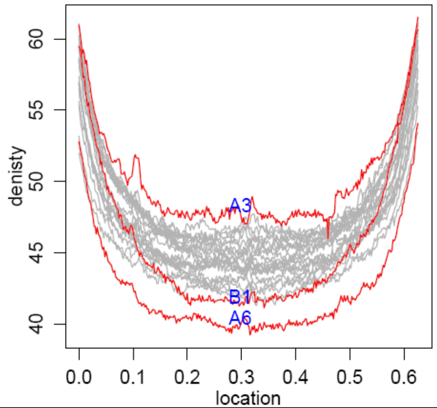
For a specified α, we could decide the upper limits.
For example, for α=10%,
Upper Limits are 2.64, 7.02, and 0.88
for these charts

Upper Limits are 2.64, 7.02, and 0.88

$$d_i = |\xi_i - \mu_\xi| / s_\xi \qquad T_m^{(1)} = \max_{1 \le j \le m} |\hat{e}_j| \qquad T_m^{(2)}(\lambda) = \sum_{j=1}^{m} |\hat{e}_j|^{\lambda}$$



Profiles A6, A3 & B1 were identified!



A6: *Lower veridical density*

A3: *Stronger local turbulence*

B1: *Most curvature*

Further Study

Underlying Model Setup

We then generate 100 individual density profiles at the chosen locations based on the following model

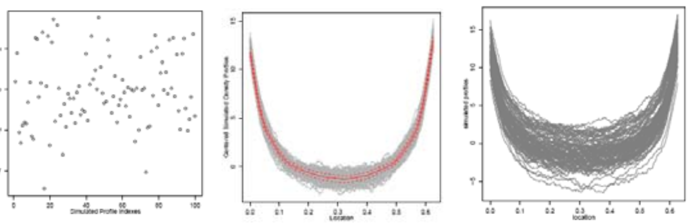
$$O_i(t) = a_i + \pi(t)^\top \alpha + e_i(t); \qquad (10)$$

where

- $\pi(t)$ is 8 dimensional quadratic B-spline basis functions with internal knots (0.06, 0.16, 0.31, 0.47, 0.56).
- a_i are i.i.d. random coefficients that follow a normal distribution $N(0, \sigma_a^2)$.
- $e_i(t)$, independent of a_i, is the error term, following a Gaussian stochastic process with constant variance and exponentially decay correlation structure, i.e.,

$$e_i(t) \sim N(0, \sigma^2); \quad \text{corr}(e_i(t), e_i(s)) = \exp\{-8|t-s|\}. \quad (11)$$

Simulation Study



Alternative Models

$$\text{Model}(a): \quad Y_i(t) = a_i + \pi(t)^\top \alpha + A\sin(10\pi t) + e_i(t),$$
$$\text{Model}(b): \quad Y_i(t) = a_i + \pi(t)^\top \alpha + B\phi(t - 0.3)/0.005 + e_i(t),$$

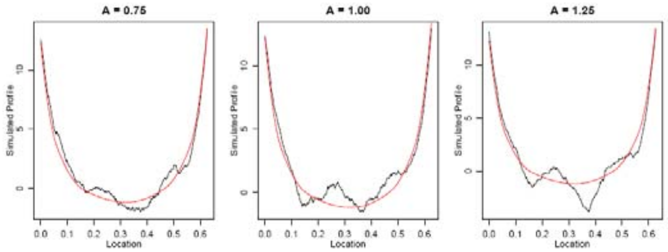
where $\phi(\cdot)$ is the density function of a standard normal.

Model (a) *represents a shape change (via magnitude A)*

Model (b) *represents a local spike (via magnitude B) while keeping the same shape.*

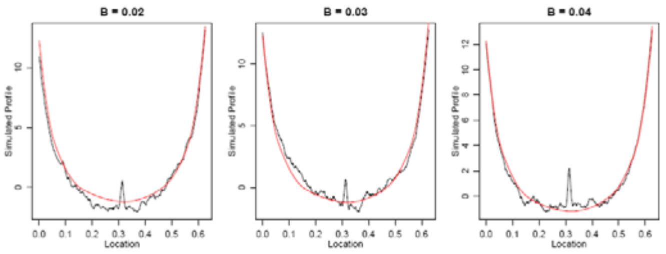
Model (a)

$$Y_i(t) = a_i + \pi(t)^\top \alpha + A\sin(10\pi t) + e_i(t)$$



Model (b)

$$Y_i(t) = a_i + \pi(t)^\top \alpha + B\phi(t - 0.3)/0.005 + e_i(t)$$



Rate of Correct Identifications

True model	Model (a)		
	$A = 0.75$	$A = 1.00$	$A = 1.25$
95%	36%	74%	100%

Model (b)		
$B = 0.02$	$B = 0.03$	$B = 0.04$
34%	82%	100%

True model	Model (a)			Model (b)		
	$A = 0.75$	$A = 1.00$	$A = 1.25$	$B = 0.02$	$B = 0.03$	$B = 0.04$
5%	36%	74%	100%	34%	82%	100%

Model Setting

$$Y_{i,j} = \xi_i + \mu(x_{i,j}) + s(x_{i,j})e_{i,j},$$

$$1 \le j \le m_i, 1 \le i \le n$$

- median$(e_{i,j}) = 0$ and median$(|e_{i,j}|) = 1$.
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What is new?

- Existing L-1 Regression
  - Independent and identical distribution (iid)
  - A longitudinal data structure
  - Time-series with restrictive dependence error structure
- A More General Class is needed here
  - A sufficiently dense measurements (vs longitudinal)
  - Could depend on both left and right neighboring measurements (vs time-series structure)

A General Class of Error Structure

$$||e_0 - e_0(j)||_q = O(\rho^j)$$

$$e_0(j) = G(\varepsilon_0, \varepsilon_{\pm 1}, \ldots, \varepsilon_{\pm j}, \varepsilon'_{\pm(j+1)}, \varepsilon'_{\pm(j+2)}, \ldots)$$

- The condition states that the contribution decays exponentially fast as j, or equivalently the distance between two measurements, increases.
- This includes m-dependent sequence, vector autoregressive moving average (VARMA) model, autoregressive conditional heteroscedastic (ARCH) model, random coefficient (RC) model, and vector nonlinear autoregressive conditional heteroscedastic (VNARCH) model.

Estimation of $\mu(x)$

- Initial estimate of $\mu(x)$

$$\hat{\mu}_{b_n}(x) = \arg\min_\theta \sum_{i=1}^{n} \sum_{j=1}^{m_i} |Y_{i,j} - \theta| K_{b_n}(x_{i,j} - x).$$

- a bias-corrected jackknife estimator

$$\tilde{\mu}_{b_n}(x) = 2\hat{\mu}_{b_n}(x) - \hat{\mu}_{\sqrt{2}b_n}(x)$$

  to remove the bias in $\hat{\mu}_{b_n}(x)$;
- we show that $\tilde{\mu}_{b_n}$ is uniformly consistent, and asymptotically normally distributed for any x.

Estimation of s(x)

- Following the estimate of $\mu(x)$, we have initial estimate $s(x)$

$$\hat{s}_{h_n}(x) = \arg\min_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{m_i} \Big| |Y_{i,j} - \tilde{\mu}_{b_n}(x)| - \theta \Big| K_{h_n}(x_{i,j} - x)$$

- an bias-corrected jackknife estimator of $s(x)$, i.e.

$$\tilde{s}_{h_n}(x) = 2\hat{s}_{h_n}(x) - \hat{s}_{\sqrt{2}h_n}(x).$$

- we also show that $\tilde{s}_{h_n}(x)$ is uniformly consistent, and enjoys asymptotic normality.

Key issues to be monitored

1. First, there might be a vertical shift, i.e., the profile may be unusually higher or lower than the normative ones.

   $\Rightarrow$ monitor the center of profiles, i.e. ξ_i's

2. Second, the shape of the new profile may different from the normative ones.

   $\Rightarrow$ Two deviation scores to monitor the shape of the profiles

Measure for Vertical Deviation

- Standardize individual profile centers:

$$d_i = |\xi_i - \mu_\xi| / s_\xi$$

— μ_ξ as the median of ξ_i's, the centers of phase I profiles,

— s_ξ as the median absolute deviation of ξ_i's

- d_i's provide a ranking of the phase I profiles from inside to the outside.
- **the screening threshold**: $(1-\alpha)$th upper quantile of the reference distribution(empirical distribution of d_i's)

Measures for Shape Deviation (1/2)

1. Centering removes the systemic distances among the profiles. Consequently, the main differences between a new centered profile Y_j and the reference curve $\mu(x)$ are mainly due to their different profile shapes.
2. Screening shape deviation based on standardized residuals

$$\hat{e}_j := \frac{Y_j - \tilde{\mu}_{b_n}(x_j)}{\tilde{s}_{h_n}(x_j)}, \quad 1 \le j \le m, \qquad ($$

Measures for Shape Deviation (2/2)

$$\hat{e}_j := \frac{Y_j - \tilde{\mu}_{b_n}(x_j)}{\tilde{s}_{h_n}(x_j)}$$

$$T_m^{(1)} = \max_{1 \le j \le m} |\hat{e}_j|, \quad \text{and} \quad T_m^{(2)}(\lambda) = \sum_{j=1}^{m} |\hat{e}_j|^{\lambda}, \quad \lambda > 0.$$

- The first statistic $T_m^{(1)}$ measures the maximal local shape deviation of the new profile from the reference profile;
- while the second score $T_m^{(2)}(\lambda)$ measures its cumulative overall shape deviation from the reference profile.
- The two scores compensate each other, and provide a comprehensive monitoring of shapes.

Theoretical Properties

To determine the screening thresholds, we first need to understand the distributions of $T_m^{(1)}$ and $T_m^{(2)}$.

- We show that, if the new profile are in the same family of the Phase I data, then
  - $T_m^{(1)}$ have an asymptotic extreme value distribution;
  - $T_m^{(2)}$ have an asymptotic normal distribution
- Both of $T_m^{(1)}$ and $T_m^{(2)}$ will converge to certain stable limiting distributions as the number of Phase I profiles goes to infinity.

Theoretical Properties

- Obtaining the thresholds directly from the limiting distribution is not easy.
- One can simply generate the reference distribution of $T^{(1)}$ and $T^{(2)}$ using the Phase I profiles.
- we calculate $T^{(1)}$ and $T^{(2)}$ for individual Phase I profiles with respect to the estimated $\tilde{\mu}_n$ and $\tilde{s}_n$, and denote them as $t_i^{(1)}$ and $t_i^{(2)}$,
- **Screening thresholds**: the $(1-\alpha)$-th quantiles of the the empirical distributions of $t_i^{(2)}$ and $t_i^{(2)}$'s.

Choices of α

$$\alpha^* = \max_{\alpha} \left\{ \alpha : \sum_{i=1}^{n} \max\{\mathbf{1}_{\{d_i > c^{(0)}(\alpha)\}}, \mathbf{1}_{\{t_i^{(1)} > c^{(1)}(\alpha)\}}, \mathbf{1}_{\{t_i^{(2)} > c^{(2)}(\alpha)\}}\} < n\alpha_0 \right\}$$

For a specified α, we could decide the upper limits.
For example, for α=10%,
Upper Limits are 2.64, 7.02, and 0.88
for these charts

Summary of the Proposed Method

Suppose (x_j, Y_j) is a new profile that is under screening,

1. we center the profile by its median $\xi = \text{median}(Y_j)$, and calculate its relative vertical deviation by $d = |\xi - \mu_\xi|/s_\xi$;
2. we then calculate the cumulative and maximal shape deviation of the centered profile, $Y_j - \xi$ with respect to $\tilde{\mu}_{b_n}(x)$ and $\tilde{s}_{h_n}(x)$.We denote the resulting shape deviation scores as $t^{(1)}$ and $t^{(2)}$.
3. if any of d, $t^{(1)}$ and $t^{(2)}$ exceeds its corresponding screening thresholds, $c^{(0)}(\alpha^*)$, $c^{(1)}(\alpha^*)$ and $c^{(2)}(\alpha^*)$, then the profile (x_j, Y_j) will be singled out.

The proposed method is theoretically validated and computationally easy!

The search of optimal bandwidth is computational expensive, but the proposed method is rather insensitive to the choice of bandwidth.

Conclusions

- Functional data is getting more and more popular.
- Treating functional data as multivariate analysis is ill-advised.
- L-1 regression is known to be robust.
- A robust control chart for monitoring functional data is proposed…it is computationally easy with solid theoretical support.
- Add to your software tools? We're on sale! Call 1-800-spc-help

A general class of nonparametric L-1 regression with its application to profile control chart

Ying Wei, Zhibiao Zhao and Dennis Lin

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