Phase I Monitoring of Nonlinear Profiles

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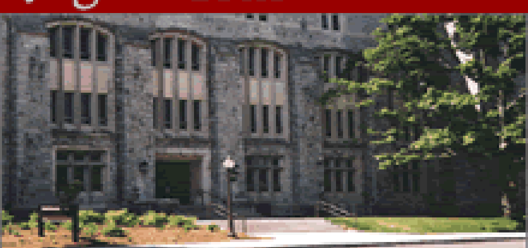


Department of Statistics

Profile Monitoring

<u>Scenario</u>

- Monitor a process or product whose quality cannot be assessed by a single quality characteristic
- Measure across some continuum (a sequence of time, space, etc.) producing a "profile"
- Various profile shapes:
  - Linear Profiles: (Kang and Albin (2000), Kim, Mahmoud, and Woodall (2003), Mahmoud and Woodall (2003))
  - Nonlinear Profiles: (Brill (2001))
- Very little work has been done to address monitoring nonlinear profiles (Woodall, *et. al.* (2003))

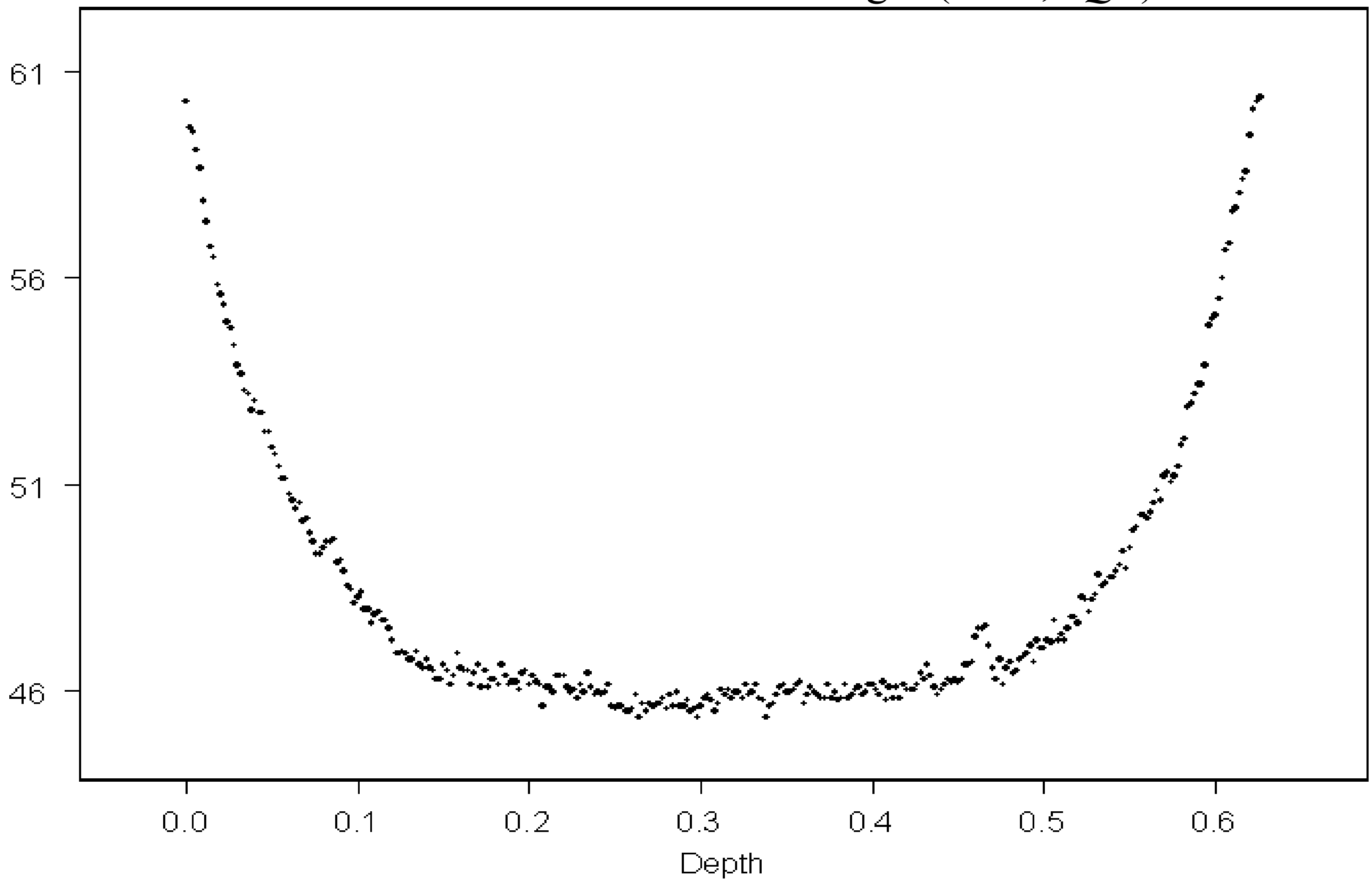
Profile Monitoring

<u>Path forward</u>

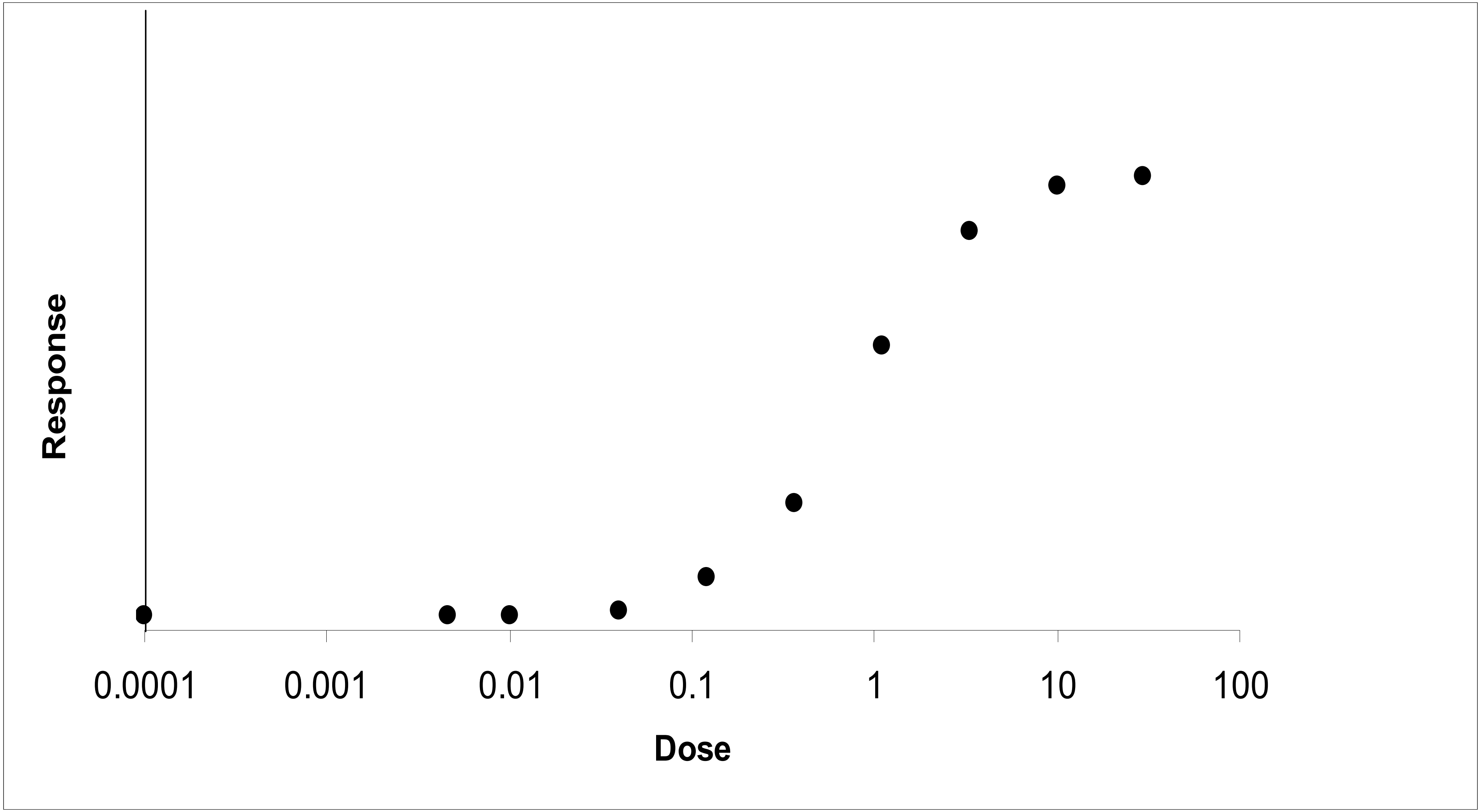
- Brill's (2001) method
- Suggest two more methods
- Illustrate methods with nonlinear profile data
- Recommendations

Example 1: Vertical Density Profile (VDP)

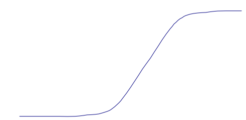
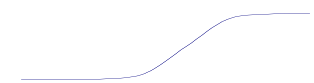
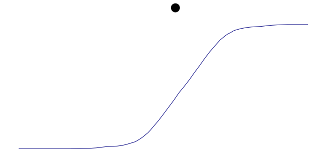
Board A1 from Walker and Wright (2002, *JQT*)



Example 2: Dose-Response Profile of a Drug



Phase I Analysis: Historical Data

		Response				Nonlinear Profile
		1	2	…	n	
Sample	1	$y_{1,1}$	$y_{1,2}$	$\cdots$	$y_{1,n}$	
	2	$y_{2,1}$	$y_{2,2}$	$\cdots$	$y_{2,n}$	
	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
	m	$y_{m,1}$	$y_{m,2}$	$\cdots$	$y_{m,n}$	

Brief Intro to Nonlinear Regression Models

Simple Case: One Y and one X

$$y_i = f(x_i, \boldsymbol{\beta}) + \varepsilon_i \qquad i = 1, \ldots, n$$

where y_i is the i^th^ response

$f(x_i, \boldsymbol{\beta})$ is an appropriate nonlinear function

x_i is the i^th^ regressor variable value

$\boldsymbol{\beta}$ is the $p \times 1$ vector of parameters to estimate

ε_i is the i^th^ residual error

Brief Intro to Nonlinear Regression Models

$\hat{\boldsymbol{\beta}}_i$ obtained iteratively for each sample

$$\hat{Var}\left(\hat{\boldsymbol{\beta}}_i\right) = \hat{\sigma}^2\left(\hat{\mathbf{D}}_i'\hat{\mathbf{D}}_i\right)^{-1} = \mathbf{C}_i$$

where $\hat{\mathbf{D}}_i$ is the estimated derivative matrix used in the estimation of the nonlinear regression parameters

Parameter Estimates from Historical Data

		Parameter			
		1	2	…	p
Sample	1	$\hat{\beta}_{1,1}$	$\hat{\beta}_{1,2}$	$\cdots$	$\hat{\beta}_{1,p}$
	2	$\hat{\beta}_{2,1}$	$\hat{\beta}_{2,2}$	$\cdots$	$\hat{\beta}_{2,p}$
	$\vdots$	$\vdots$	$\vdots$		$\vdots$
	m	$\hat{\beta}_{m,1}$	$\hat{\beta}_{m,2}$	$\cdots$	$\hat{\beta}_{m,p}$

How to Monitor Nonlinear Profiles

- Ideally, monitor each parameter independently
- Problem: parameter estimates are correlated in nonlinear regression
- Cannot monitor each parameter separately, so use a multivariate T^2 control chart to monitor the parameters simultaneously

Multivariate T^2 Control Chart Statistic

General form of the T^2 statistic:

$$T_i^2 = \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)' \mathbf{S}^{-1} \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right) \qquad i = 1, \ldots, m$$

$\mathbf{S}$ is the covariance matrix of parameter estimates

$$\hat{\boldsymbol{\beta}}_i = \begin{pmatrix} \hat{\beta}_{i,1} \\ \hat{\beta}_{i,2} \\ \vdots \\ \hat{\beta}_{i,p} \end{pmatrix} \qquad \overline{\hat{\boldsymbol{\beta}}} = \begin{pmatrix} \frac{1}{m}\sum_{i=1}^{m} \hat{\beta}_{i,1} \\ \frac{1}{m}\sum_{i=1}^{m} \hat{\beta}_{i,2} \\ \vdots \\ \frac{1}{m}\sum_{i=1}^{m} \hat{\beta}_{i,p} \end{pmatrix}$$

Three Choices for S

Method 1: Sample Covariance Matrix (Brill, 2001)

$$\mathbf{S}_1 = \frac{1}{m-1}\sum_{i=1}^{m}\left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)\times\left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)'$$

<u>Pros</u>:
- Easy to calculate
- Widely used and easily understood

<u>Cons</u>:
- Greatly affected by shifts in mean vector
- Results in low power for the T^2 control chart

Three Choices for S

Method 2: Successive Differences (Holmes and Mergen, 1993)

Let $\mathbf{v}_i = \hat{\boldsymbol{\beta}}_{i+1} - \hat{\boldsymbol{\beta}}_i \qquad i = 1, \ldots, m-1$

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}'_1 \\ \mathbf{v}'_2 \\ \vdots \\ \mathbf{v}'_{m-1} \end{bmatrix} \qquad \text{Then} \qquad \mathbf{S}_2 = \frac{\mathbf{V}'\mathbf{V}}{2(m-1)}$$

<u>Pros</u>:
- Like moving range with individual observations
- Not effected by shifts in the mean vector
- High power

<u>Cons</u>:
- Less statistical theory developed to date

Three Choices for S

Method 3: Intra-Profile Pooling

For each of the *m* samples: $$\hat{Var}\left(\hat{\boldsymbol{\beta}}_i\right) = \hat{\sigma}^2\left(\hat{\mathbf{D}}_i'\hat{\mathbf{D}}_i\right)^{-1} = \mathbf{C}_i$$

Then $$\mathbf{S}_3 = \frac{1}{m}\sum_{i=1}^{m}\mathbf{C}_i$$

Pros:
- Uses information from nonlinear regression estimation

Cons:
- Does not account for profile-to-profile common cause variability

Three Choices for T_i^2

Three formulations of the T^2 statistic:

Method 1: Sample Covariance Matrix

$$T_{1,i}^2 = \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)' \mathbf{S}_1^{-1} \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)$$

Method 2: Successive Differences

$$T_{2,i}^2 = \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)' \mathbf{S}_2^{-1} \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)$$

Method 3: Intra-Profile Pooling

$$T_{3,i}^2 = \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)' \mathbf{S}_3^{-1} \left(\hat{\boldsymbol{\beta}}_i - \overline{\hat{\boldsymbol{\beta}}}\right)$$

Upper Control Limits

Method 1: Sample Covariance Matrix

$$T_1^2 \frac{m}{(m-1)^2} \sim Beta\left(\frac{p}{2}, \frac{m-p-1}{2}\right)$$

As discussed by Sullivan and Woodall (1996)

$$UCL_1 = \frac{(m-1)^2}{m} B_{1-\alpha, p/2, (m-p-1)/2}$$

Upper Control Limits

Method 2: Successive Differences

Approximately $T_2^2 \frac{m}{(m-1)^2} \sim Beta\left(\frac{p}{2}, \frac{f-p-1}{2}\right)$

where $f = \frac{2(m-1)^2}{3m-4}$

For more information, see Scholz and Tosch (1994)

$$UCL_2 = \frac{(m-1)^2}{m} B_{1-\alpha, p/2, (f-p-1)/2}$$

Upper Control Limits

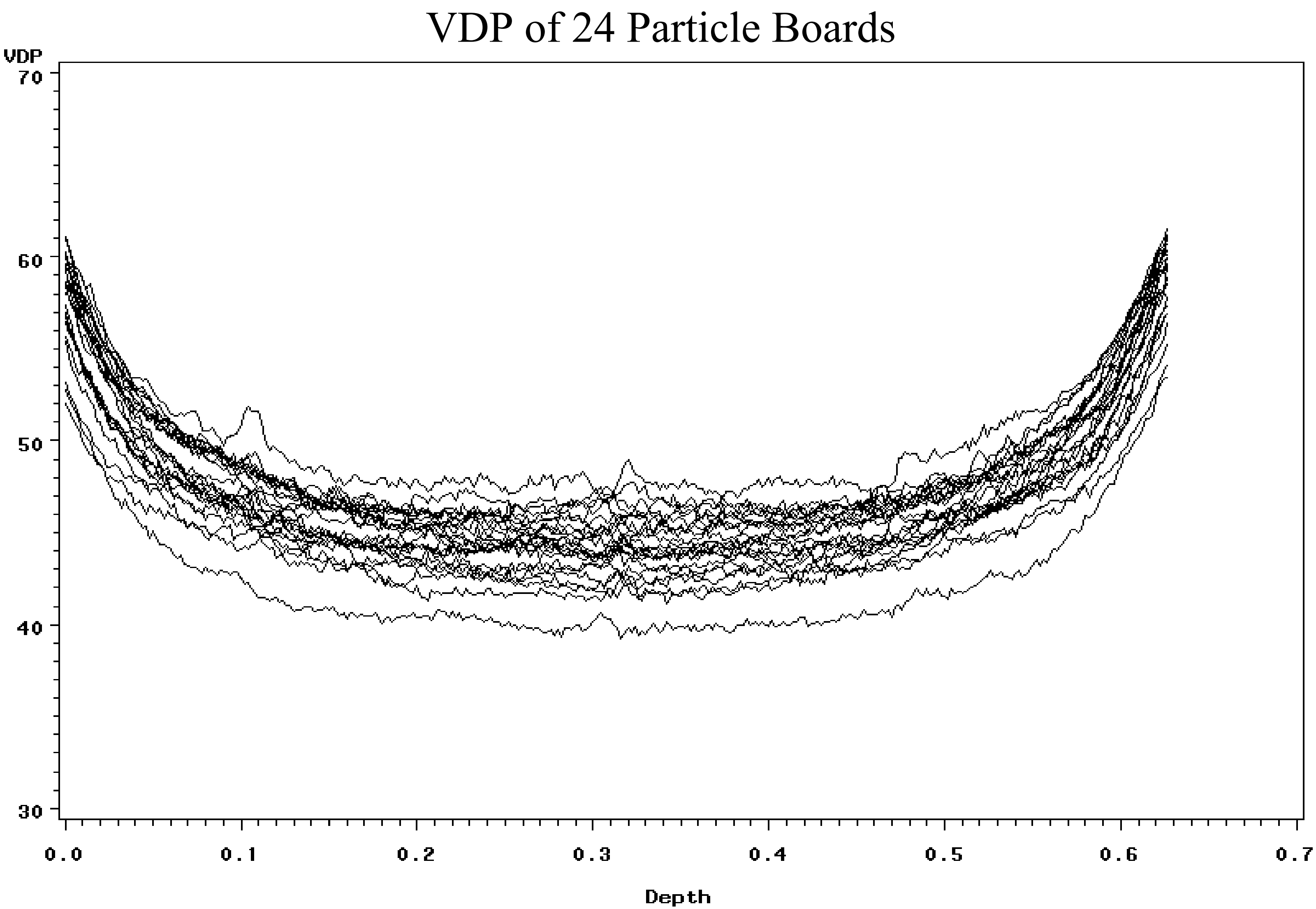
Method 3: Intra-Profile Pooling

We think that approximately $$T_3^2 \frac{m(m-p)}{p(m-1)(m+1)} \sim F(p, m-p)$$

$$UCL_3 = \frac{m(m-p)}{p(m-1)(m+1)} F_{1-\alpha, p, m-p}$$

Control limits are best approximations so far

Illustration: VDP Data



Nonlinear Function to Model VDP Data

Use a "bathtub" function to model each board from the VDP data

$$f(x_i, \boldsymbol{\beta}) = \begin{cases} a_1(x_i - d)^{b_1} + c & x_i > d \\ a_2(-x_i + d)^{b_2} + c & x_i \le d \end{cases}$$

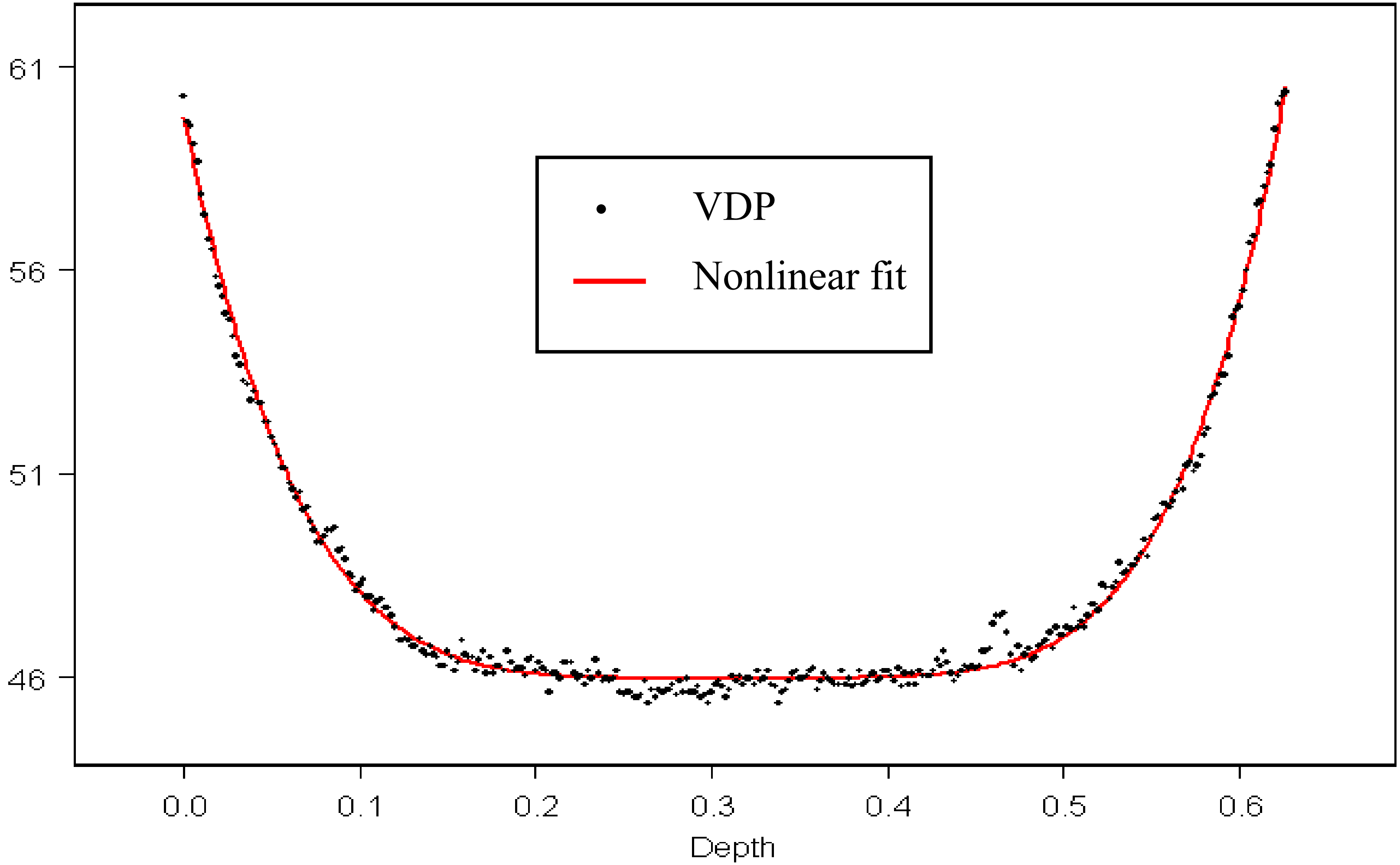
where x_i is the i^th regressor variable value

$$\boldsymbol{\beta} = \begin{pmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \\ c \\ d \end{pmatrix}$$

- a_1, a_2 } determine the width of the "bathtub"
- b_1, b_2 } determine the "flatness" of the "bathtub"
- c → is the bottom of the "bathtub"
- d → is the center of the "bathtub"

Nonlinear Function to Model VDP Data

Board #1 from Walker and Wright (2002, *JQT*)



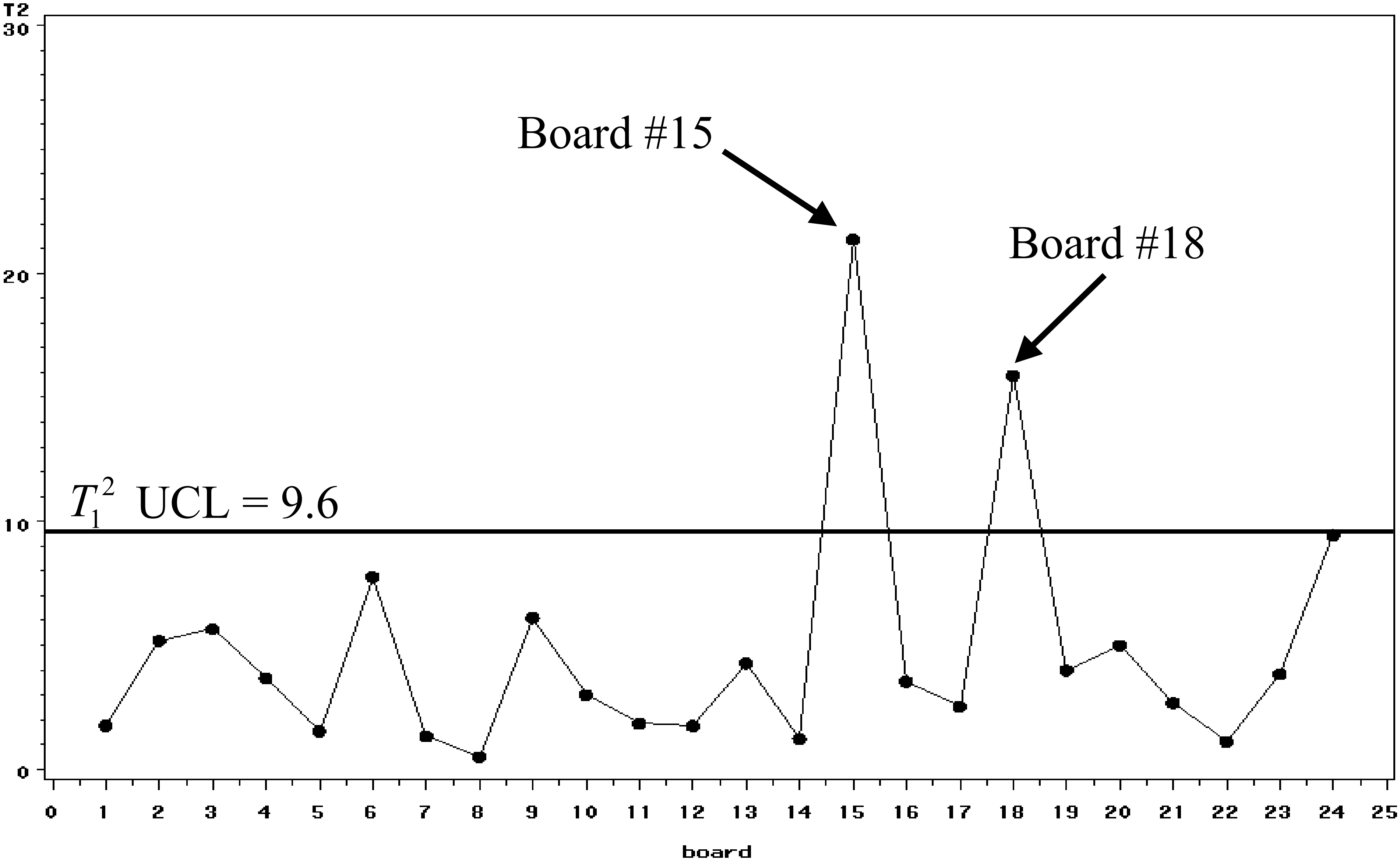
Nonlinear Function to Model VDP Data

Estimated nonlinear profile of Board #1

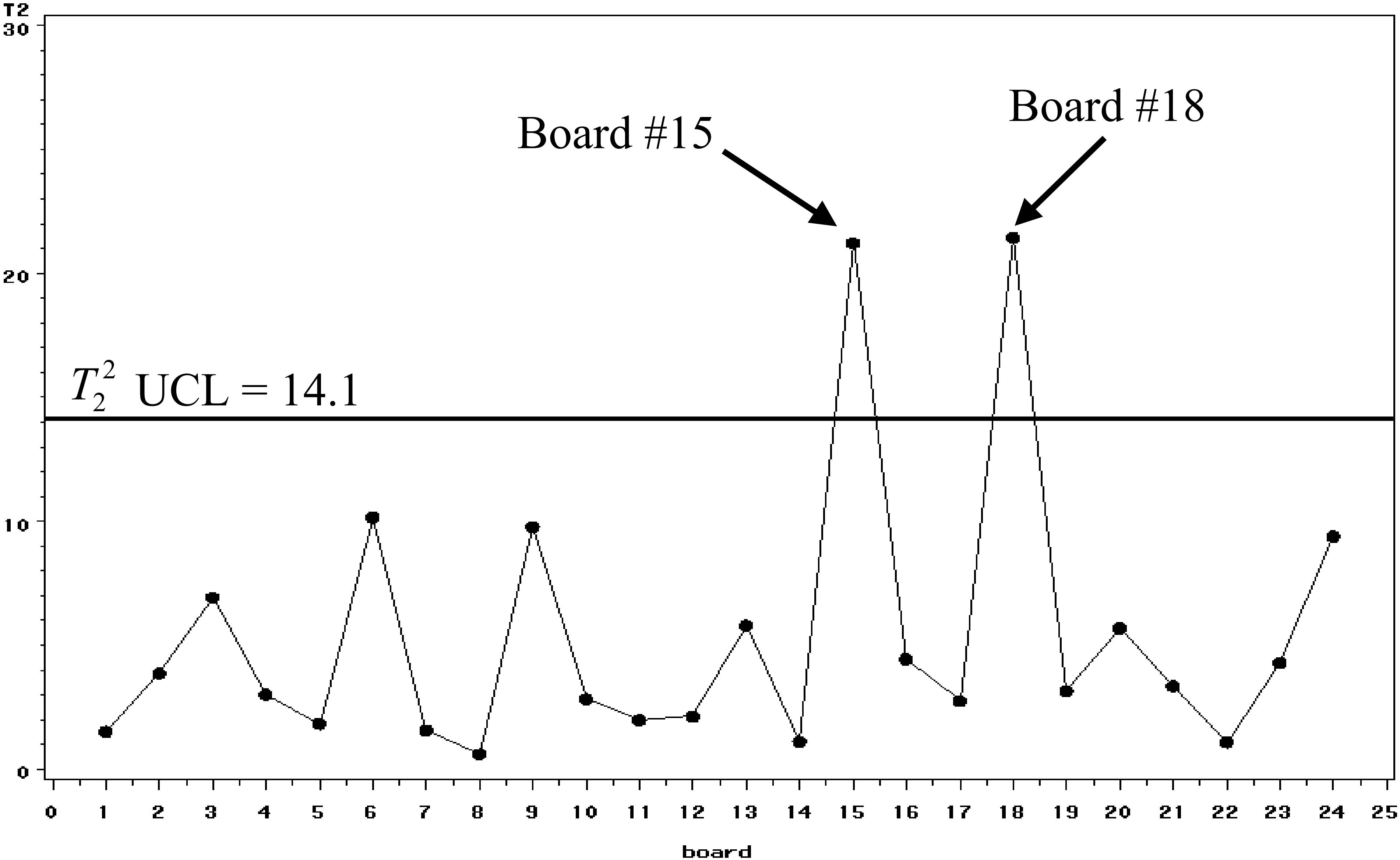
$$f(x_i, \hat{\boldsymbol{\beta}}) = \begin{cases} 5708(x_i - 0.313)^{5.14} + 46.0 & x_i > 0.313 \\ 3921(-x_i + 0.313)^{4.87} + 46.0 & x_i \le 0.313 \end{cases}$$

- Estimate profile for each board
- Calculate $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_{3.}$
- Calculate T_1^2, T_2^2, and T_3^2

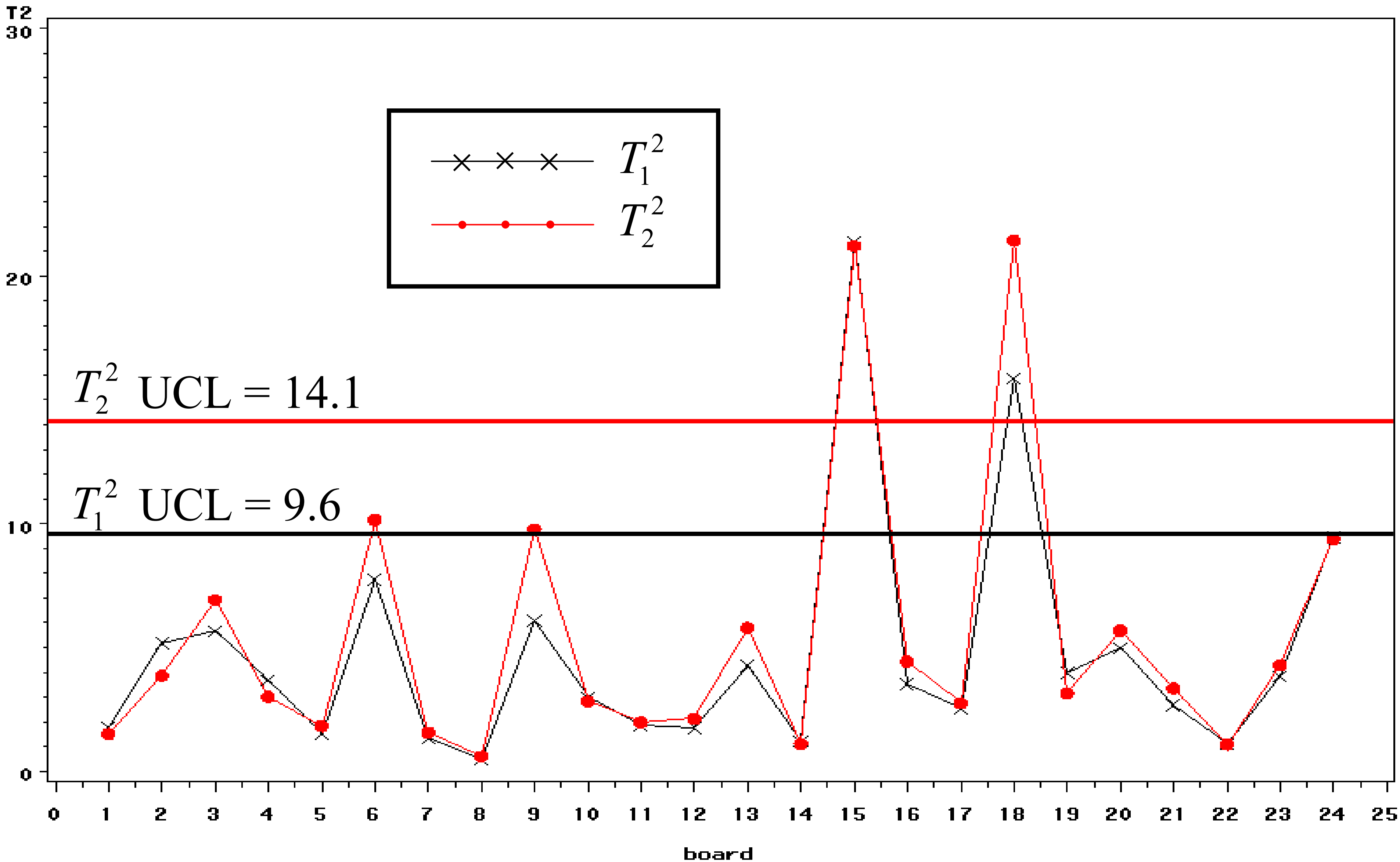
T_1^2 Control Chart



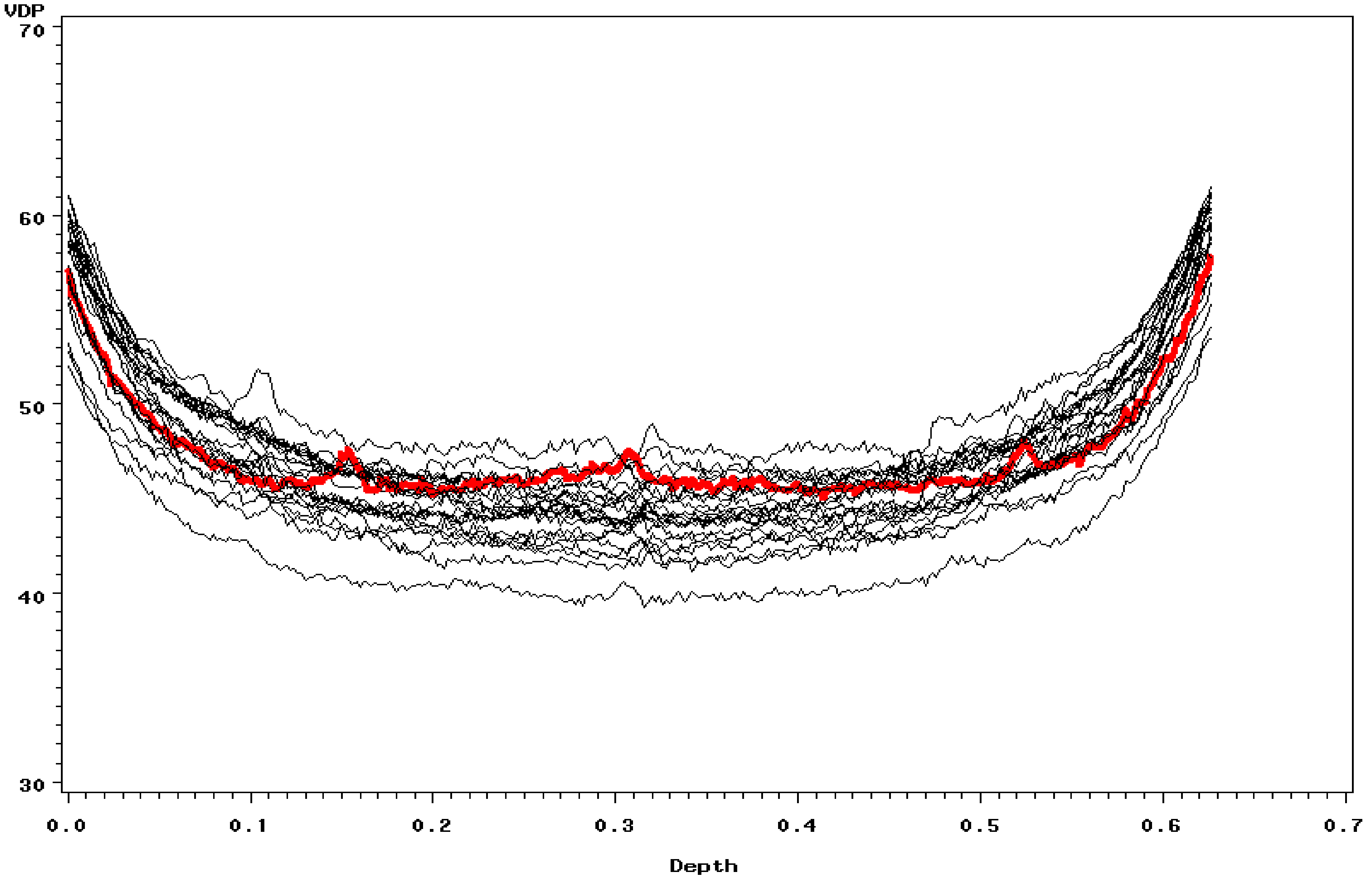
T_2^2 Control Chart



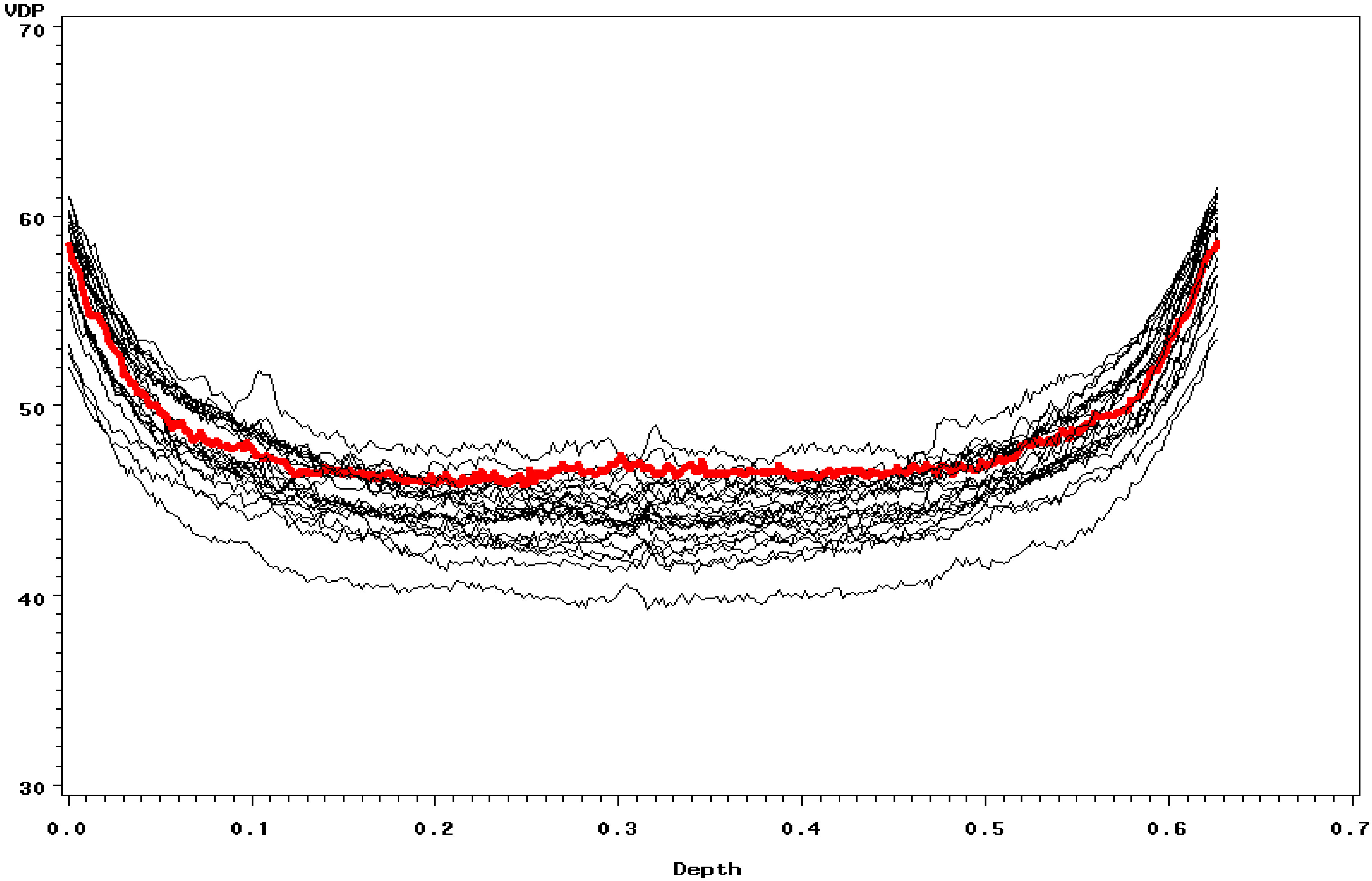
T_1^2 and T_2^2 Control Charts



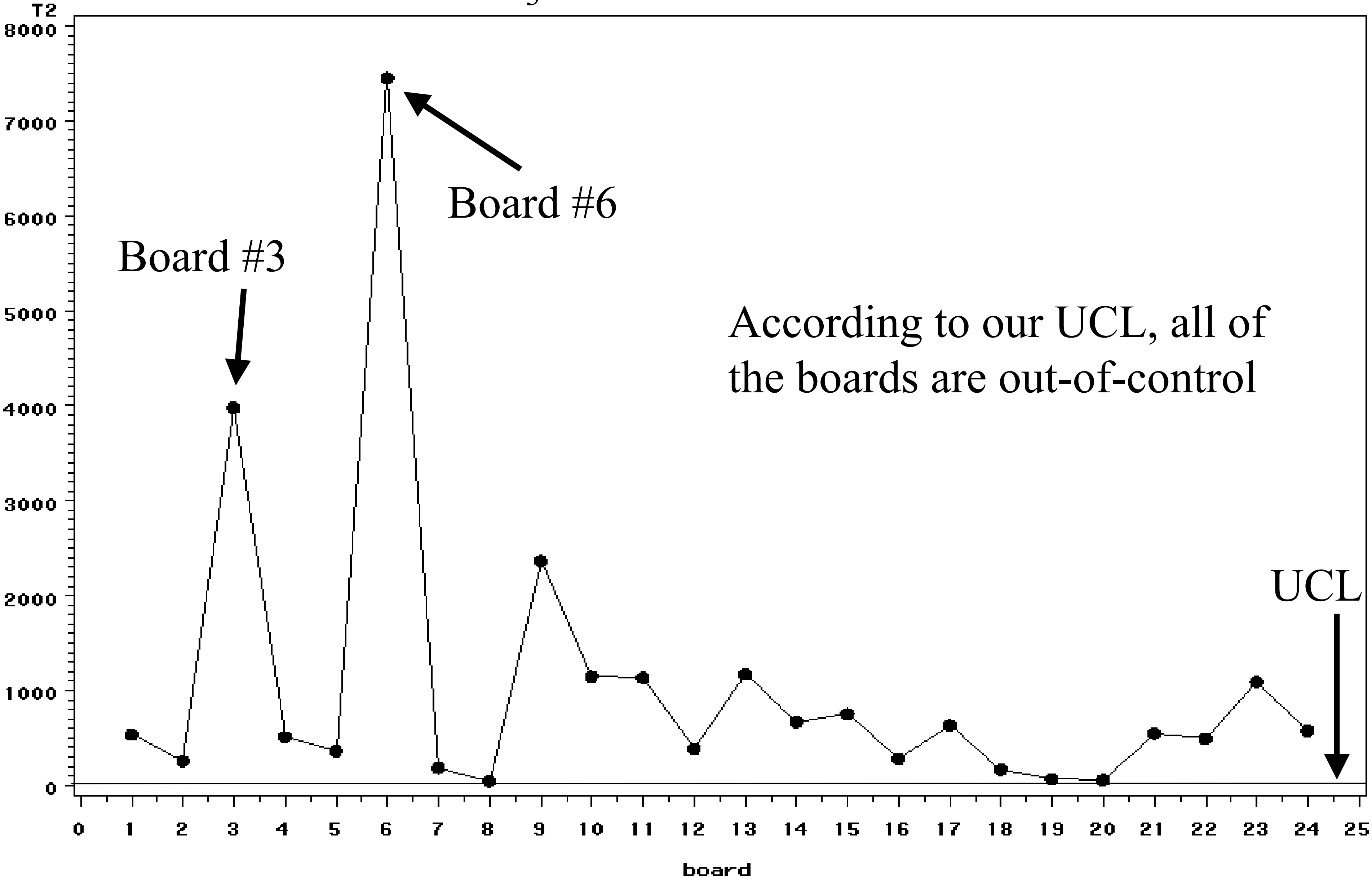
Board 15



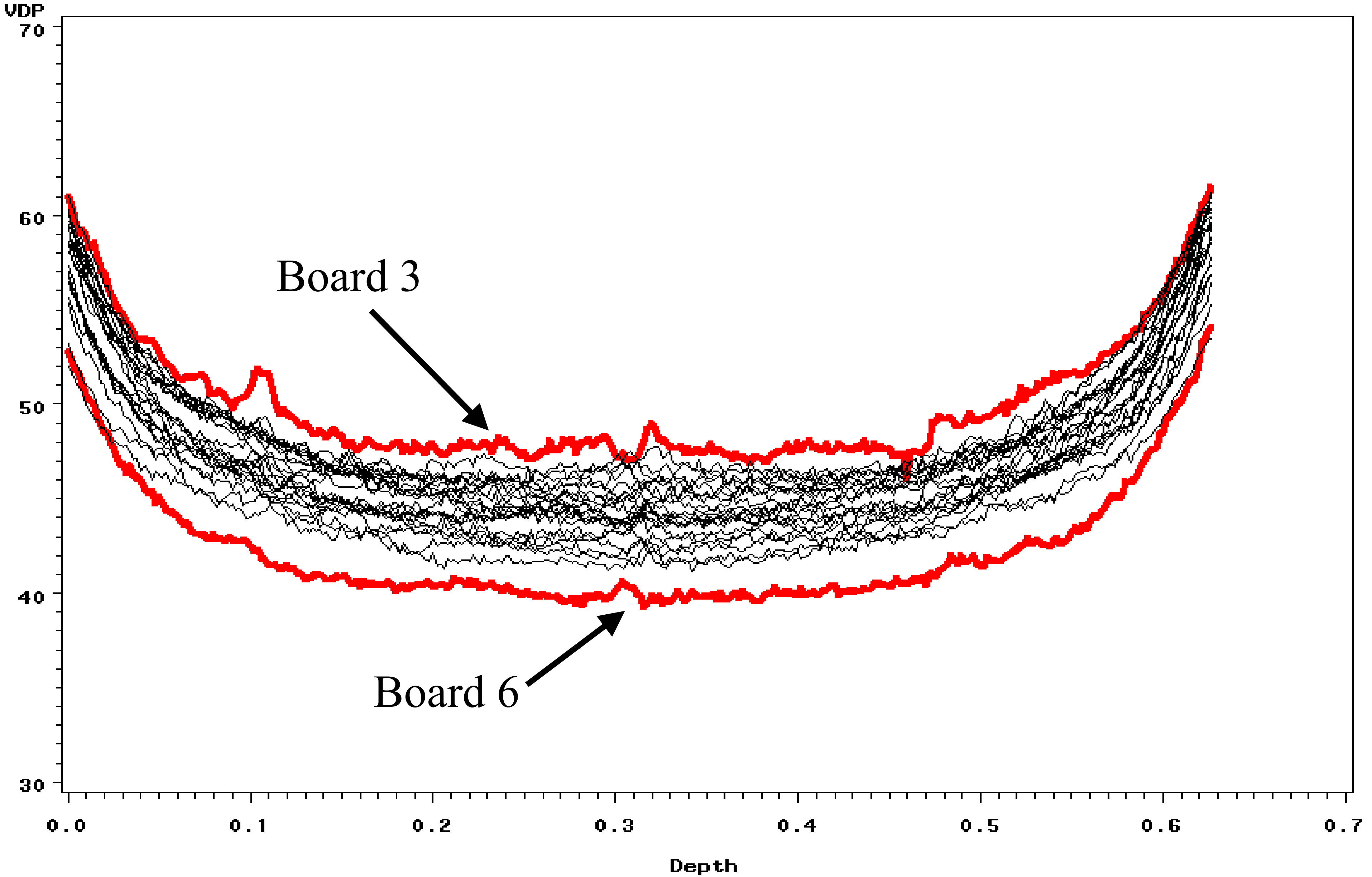
Board 18



T_3^2 Control Chart



Boards 3 and 6



Conclusions

- Method 1 (sample covariance matrix) does not take into account the sequential sampling structure of the data:
  - The overall probability of detecting a shift in the mean vector will decrease (See Sullivan and Woodall, 1996)
  - Should not be used
- Method 2 (successive differences) accounts for the sequential sampling scheme, and gives a more robust estimate of the covariance matrix
- In the VDP example, both Methods 1 and 2 gave same result because
  - No apparent shift in the mean vector
  - There were only about two outliers

Conclusions

- Method 3 (intra-profile pooling) should be used when there is no profile-to-profile common cause variability
- Comparison of the three methods:
  - Method 1 assumes all variability is due to common cause
  - Method 3 assumes that no variability is due to common cause
  - Method 2 is somewhere in the middle

Issue: Monitoring parameters versus monitoring the fitted curves

References

Brill, R. V. (2001). "A Case Study for Control Charting a Product Quality Measure That is a Continuous Function Over Time". Presentation at the 45th Annual Fall Technical Conference, Toronto, Ontario.

Holmes, D. S., and Mergen, A. E. (1993). "Improving the Performance of the T^2 Control Chart". *Quality Engineering* **5**, pp. 619-625.

Kim, K., Mahmoud, M. A., and Woodall, W. H. (2003). "On The Monitoring of Linear Profiles". To appear in the *Journal of Quality Technology*.

Mahmoud, M. A., and Woodall, W. H. (2003), "Phase I Monitoring of Linear Profiles with Calibration Applications", Submitted to *Technometrics*.

Scholz, F. W., and Tosch, T. J. (1994), "Small Sample Uni- and Multivariate Control Charts for Means". *Proceedings of the American Statistical Association, Quality and Productivity Section*.

Sullivan, J. H., and Woodall, W. H. (1996), "A Comparison of Multivariate Quality Control Charts for Individual Observations". *Journal of Quality Technology* **28**, pp. 398-408.

Walker, E., and Wright, S. P. (2002). "Comparing Curves Using Additive Models". *Journal of Quality Technology* **34**, pp. 118-129.

Woodall, W. H., Sptizner, D. J., Montgomery, D. C., and Gupta, S. (2003). "Using Control Charts to Monitor Process and Product Profiles". Submitted to the *Journal of Quality Technology*.