A Yokogawa Commitment to Industry

vigilance™

Data Reconciliation Techniques

By using a NIR Analyzer with Chemometrics Software in Fuel Property Analysis.

Santanu Talukdar

Manager, Engineering Services

Data Reconciliation Techniques

Part 1

References

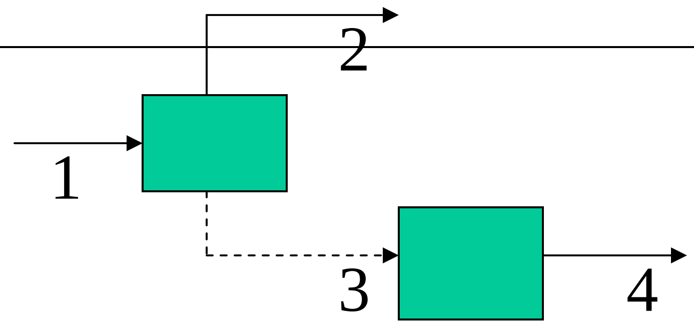
Topics on Data Reconciliation is based on works of V.V. Veverka & F.Madron

Acknowledgements

A Yokogawa Commitment to Industry
vigilance™.

Yokogawa Corporations India & Japan

Data Reconciliation



F1 – F2 – F3 = 0

F3 – F4 = 0

$$\boxed{F(\underline{x}\, ,\, \underline{y}\, ,\, \underline{c}) = 0}$$

X – Measured

Y – Unmeasured

C - Constant

$$\boxed{xi^{+} = xi + ei}$$

xi – Measured Data

ei –Error Characterized by SD σ

Measured
- Redundant – Can be calculated from other measured variable
- Non-redundant

Unmeasured
- Observable – Can be uniquely calculated from other measured variable
- Non-observable

For Redundant Systems

$$f(\underline{x}, \underline{y}, \underline{c}) \neq 0$$

$$\hat{x}, \hat{y}$$

$$f(\underline{\hat{x}}, \underline{\hat{y}}, \underline{\hat{c}}) = 0$$

and

$$\hat{X} = \Sigma \left(\frac{xi - x +}{\sigma} \right)^2 \quad => \min$$

Least Sq. Soln.

Reconciled Value

For redundant Systems

$$\frac{\sigma \text{ reco}}{\sigma \text{ meas}} \leq \mathbf{1}$$

Reconciliation

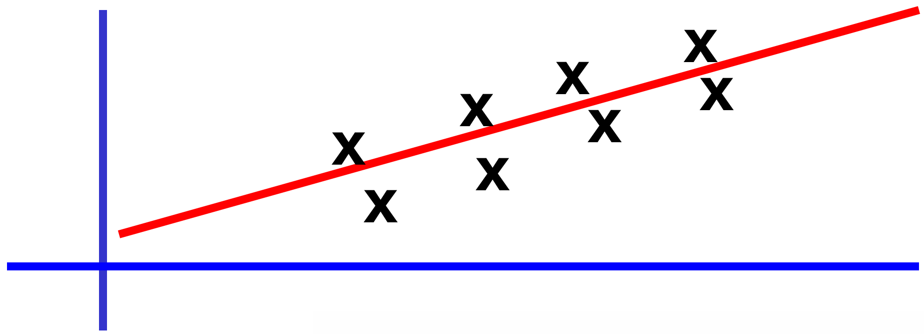
↓

Provides Info

↓

•Possible Gross Errors
•Accuracy of Results
•Propagation of Measurement Errors

Regression / Reconciliation



Regression ⟷ Reconciliation

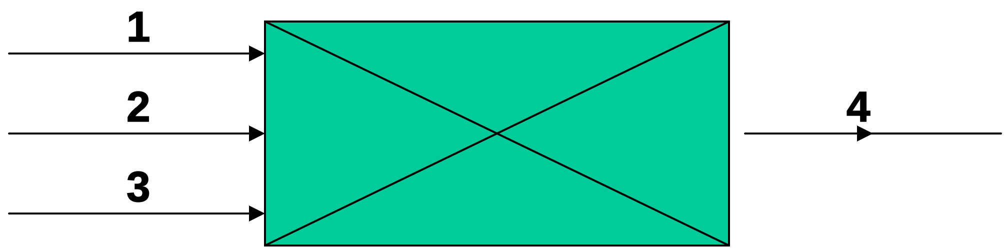
Regression	Reconciliation
Data reconciled on least Squares (Measured data)	Data reconciled on least Squares (Measured data)

Parameter Estimation	Propagation of Measurement Error
Reconciliation	
Gross Error Elimination	Measurement Design

Following are the Special Cases of Reconciliation:

- Classical Balancing
- Simulation
- Regression

Applications in Blending



Static Mixer

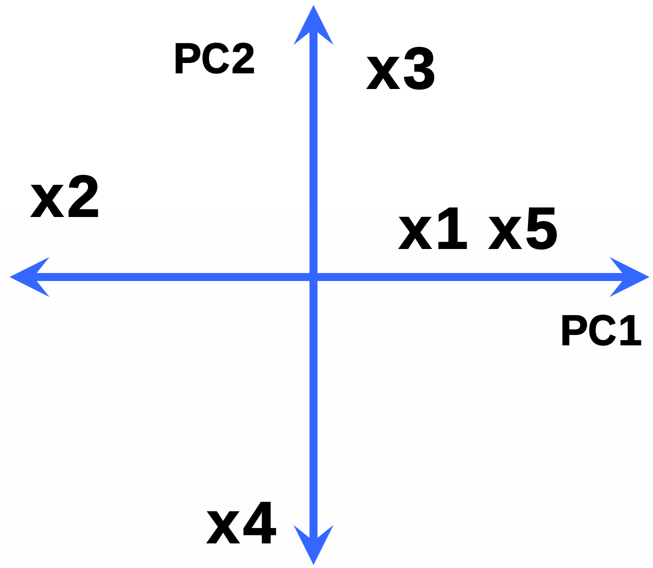
$$F_1 + F_2 + F_3 - F_4 = 0$$

(Mass Balance on Measured / Observed Data)

Gross Error Detection thru Outlier Defination By Principal Component Analysis (PCA)

A Yokogawa Commitment to Industry vigilance™

Loading Plot



Case 1 : Variables x1 & x2 are negatively correlated

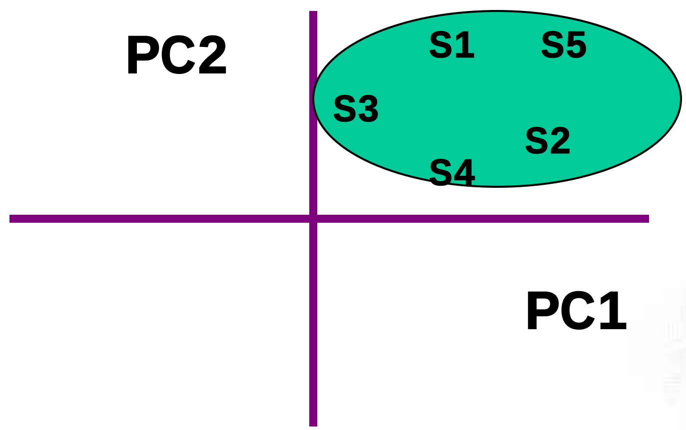
Case 2 : Variables x1 & x5 are positively correlated

Case 3 : Variables x3 & x4 are negatively correlated.

- The Variables are plotted on two orthogonal axes, Principal components 1 and 2 known as PC1 and PC2
- Case 3 Type Variables will not influence on Case 1 and Case 2 Variables

Interrelations between Samples & Variables determined by Score Plot – Sample Cluster 1

	x1	x2	x3	x4	x5
S1	H	L			H
S2	H	L			H
S3	H	L			H
S4	H	L			H
S5	H	L			H

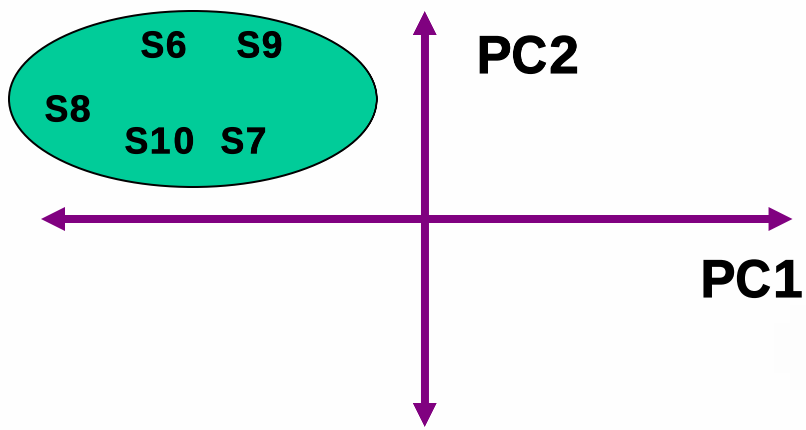


Sample Cluster 1

For all samples lying to the right of the Plot, the variables x1 and x5 will be high

Interrelations between Samples & Variables determined by Score Plot – Sample Cluster 2

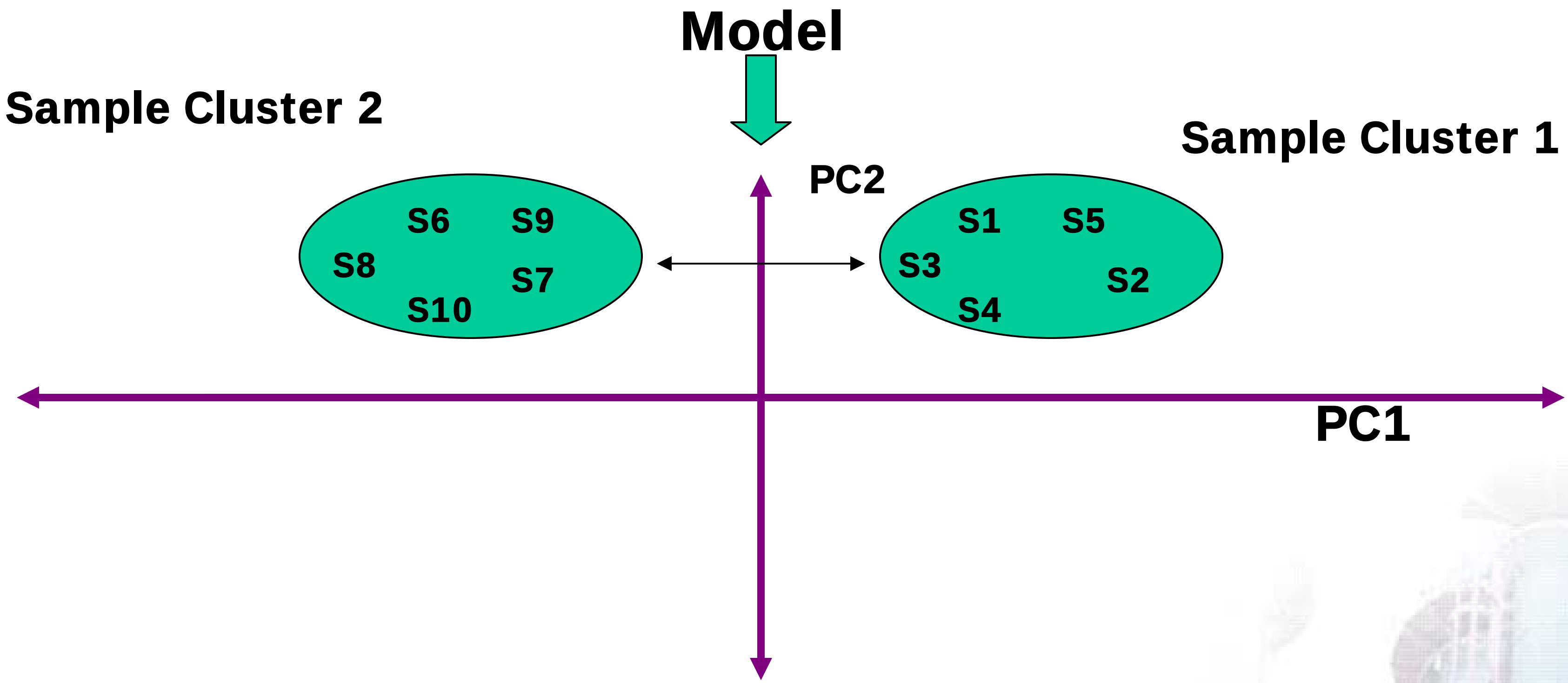
	x1	x2	x3	x4	x5
S6	L	H			L
S7	L	H			L
S8	L	H			L
S9	L	H			L
S10	L	H			L



Sample Cluster 2

For all samples lying to the left of the Plot, the variables x2 only, will be high

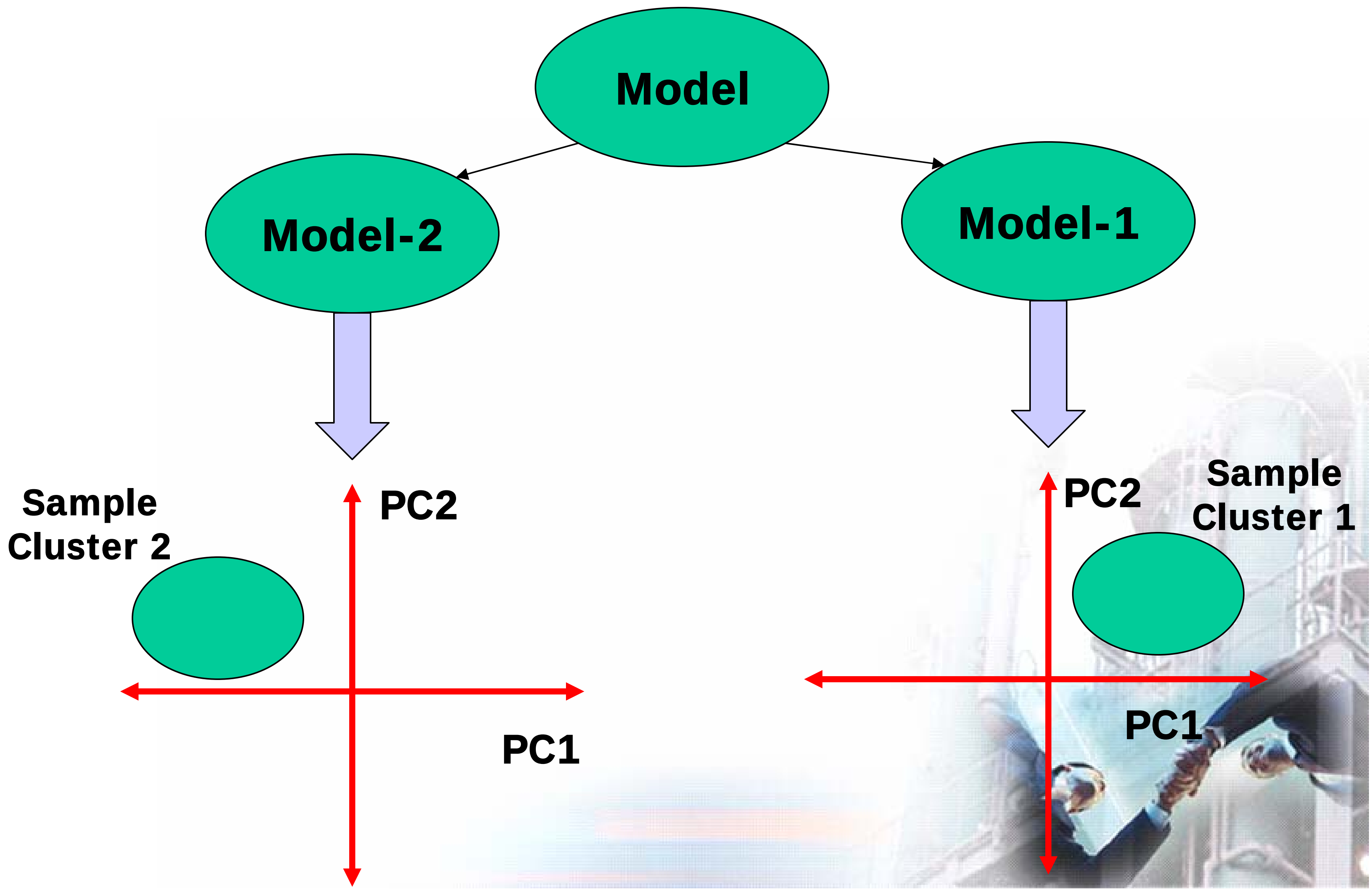
Gross Error Detection



- These two sample clusters are outlying to each other.
- Outliers are a major cause of Gross Errors

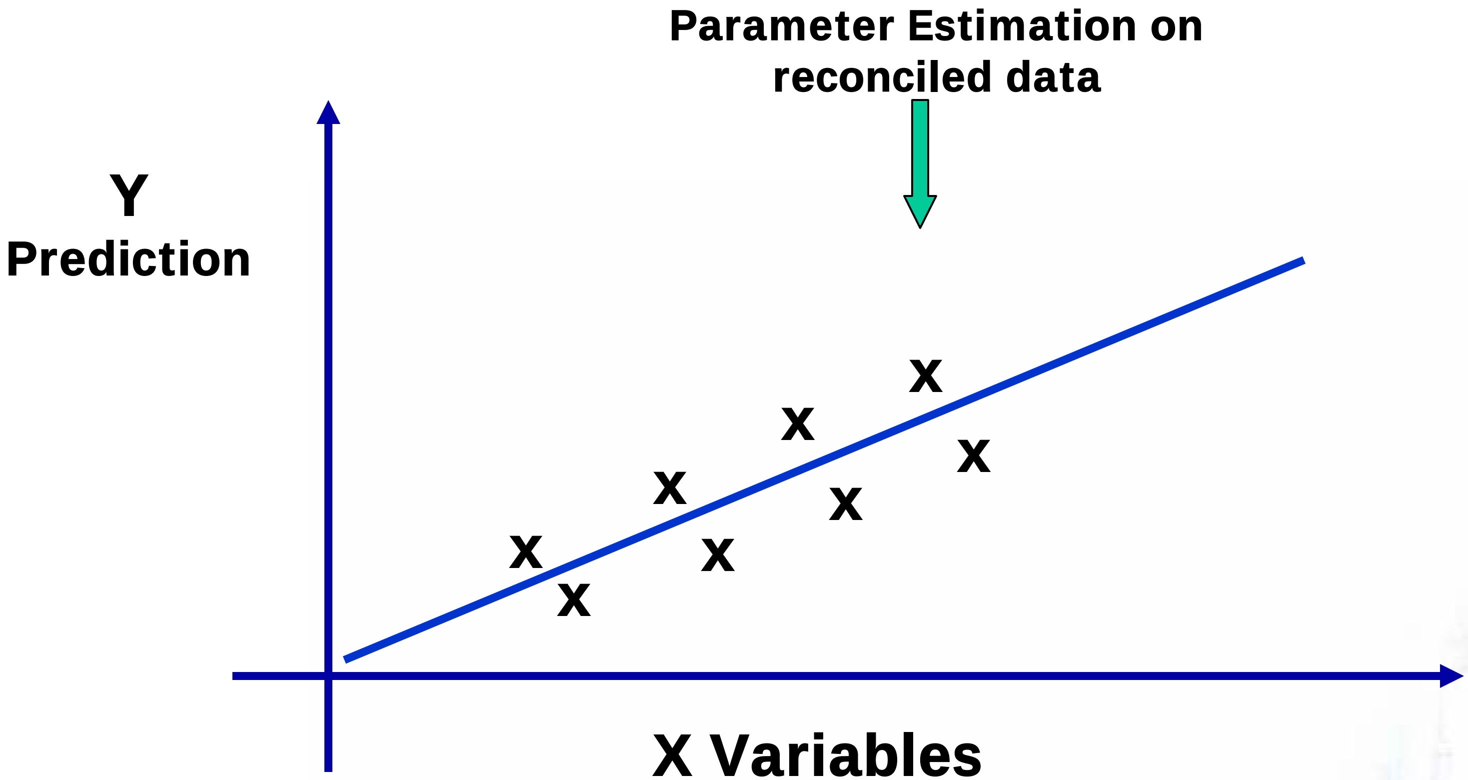
Gross Error Elimination
through Outlier Elimination

Data Reconciled thru' Gross Error Elimination by removal of Outliers



Data Reconciliation – Step 1

Step 1



Step 1:

Regression performed on reconciled data from a sample set of known values (Measured Y / Known X).
Regression performed by least square techniques

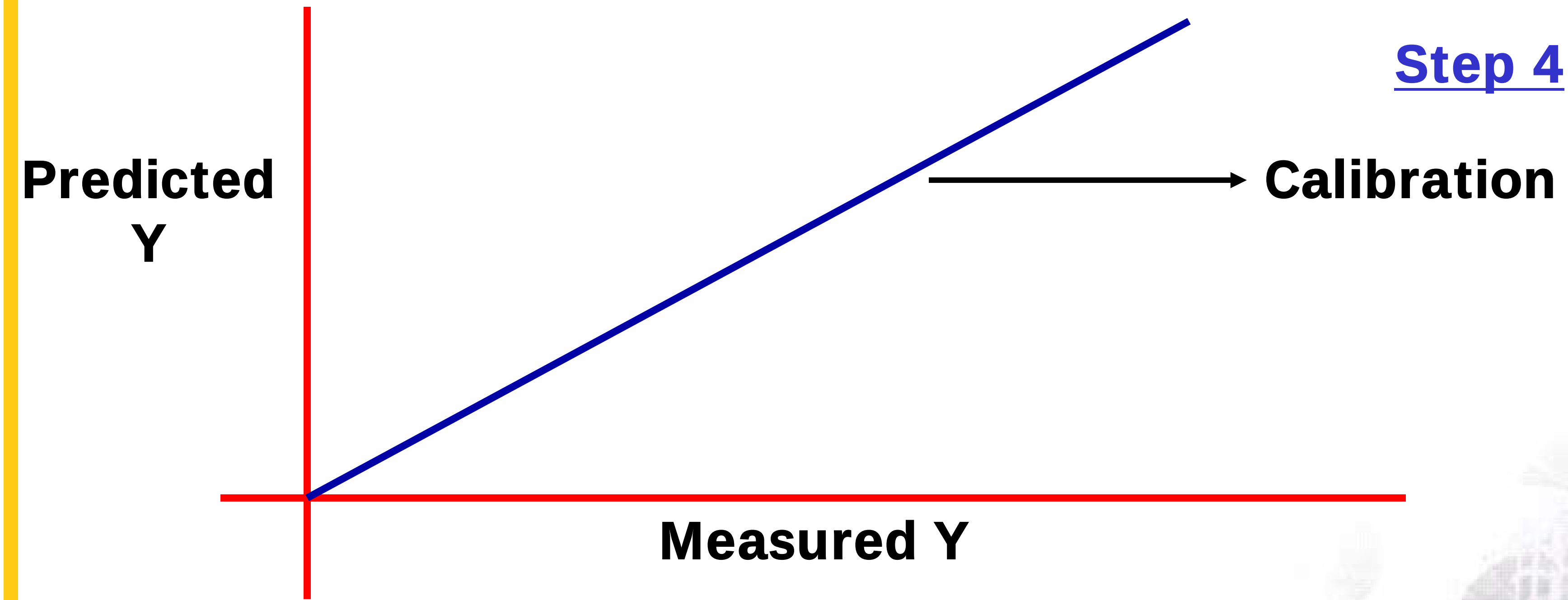
Step 2 :

Regression Co-efficients are calculated

Step 3 :

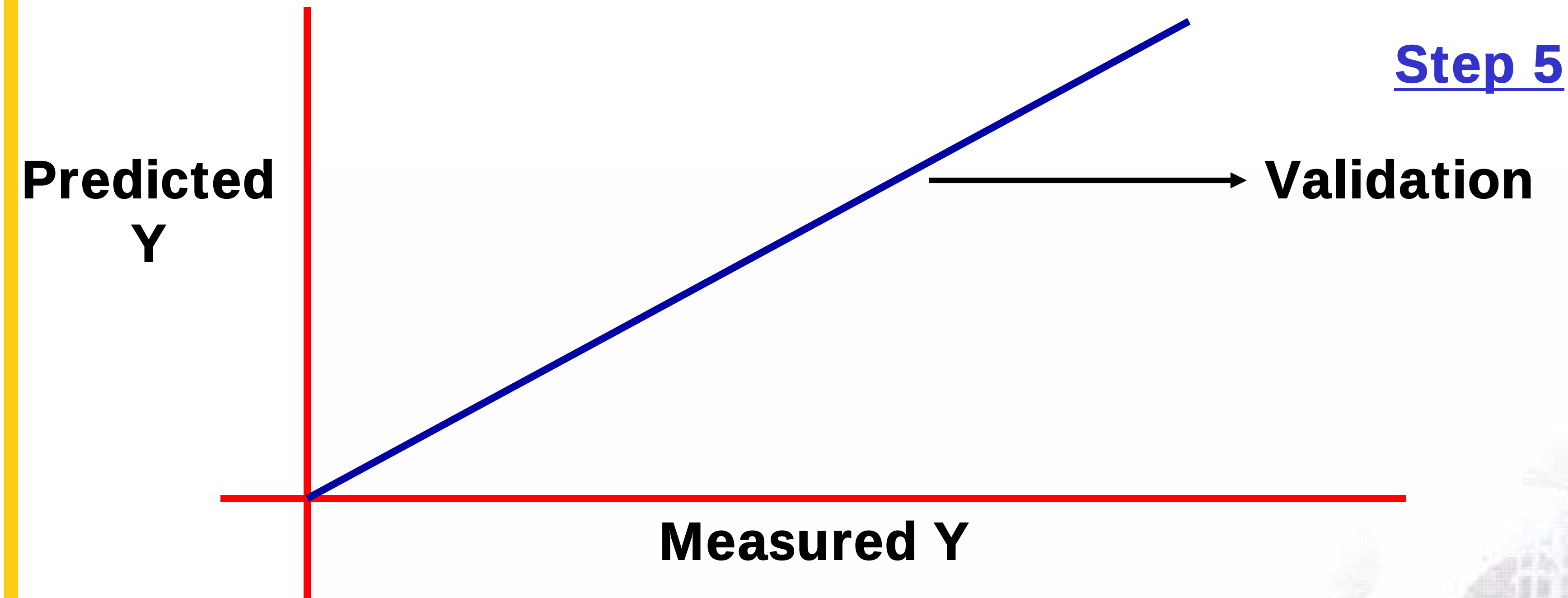
Calibration is performed from these calculated co-efficient to generate predictions (Predicted Y)

Step 4



The regressed line is tabulated on Measured Y v/s Predicted Y. SD error is RMSEC.

Data Reconciliation – Step 5



The Calibrated Model is validated on the known sample set by Cross-validation technique.

SD error is RMSEV.

Step 6

Unknown Sample from similar sample population is predicted from the Calibration Set.

A Yokogawa Commitment to Industry vigilance™

Gross error can also generate due to: Step 7

1. Process leaks. Typical is measurement design constraint as :
   - Crude Type
   - Energy Effcy
   - Separation Effcy
   - Treatment Effcy
   - Catalytic and Rxns Effcy

Gross error can also generate due to:

Step 7

2. Propagation of Measurement Error as :

Elementary Error → Errors of Primary Variables → Errors of Secondary Variables

Error of Cold End of TC → Error of Temperature → Error of Flow

Ref. F.Madron, Data Reconciliation.

Data Reconciliation thru' Gross Error Elimination – Step 8

To Eliminate gross errors in Steps 1 – 5, number of samples in a set should be large enough to be statistically significant

Step 8

Conclusion :

Gross Errors

↓

Cause Outliers

↓

Outliers happen due to

↓

- **Process Leaks**
- **Propagation of Measurement Errors**

- **Different sample clusters due to different sample population**
- **Example : Change in blend recipe**

Benefits :

A Yokogawa Commitment to Industry

•NIR repeatability < / = 2 x RMSE < / = ASTM repeatability.

•NIR can achieve lower blending target octane numbers than traditional ASTM analyzers.

•Outlier alarm can be triggered if NIR value exceeds the threshold value of Blend target values.

•Process operators can take action to analyze outliers.

•Leads to predicted tank quality estimation.

•Saves on tank reblend.

•Saves on repeated manual analysis for final property values; multiple physical property analysis within scan time of few minutes

•Fast control decision if interfaced in control loop.

•Cost savings to users. NIR as a process optimization can lead to six sigma process control.

•OPEX reduction thru' improvements in 3Es (Energy, Environment, Emissions).

Thank you very much for your attention.

Comments : ?

E-mail : Santanu.Talukdar@in.yokogawa.com

A Yokogawa Commitment to Industry

vigilance™