Statistics for Engineering

Section 6: Latent variable modelling

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What we will cover

- What is a latent variable?
- Applications of latent variable methods

Extracting value from data

Ankit - 4C3 student in 2010 - now at Tenova:

- *Now, having worked for over a year, I find myself referring back to my notes all the time and appreciating the concepts about how to look at data and represent the data in the best possible manner, especially since on a daily basis I look at a gigantic amount of data and am required to make sense of it.*

- *I think what I loved most about the course was the emphasis on the* **thinking** *and* **process of getting to a solution** *instead of the the final solution itself which has been an important attribute to becoming a good engineer or a problem solver/troubleshooter.*

Extracting value from data

Engineers deal with large quantities of data from many different sources. We can do some some interesting *and profitable* things with these data:

1. Improve process understanding
2. Troubleshooting process problems
3. Improving, optimizing and controlling processes
4. Predictive modelling (inferential sensors)
5. Process monitoring

What is a latent variable?

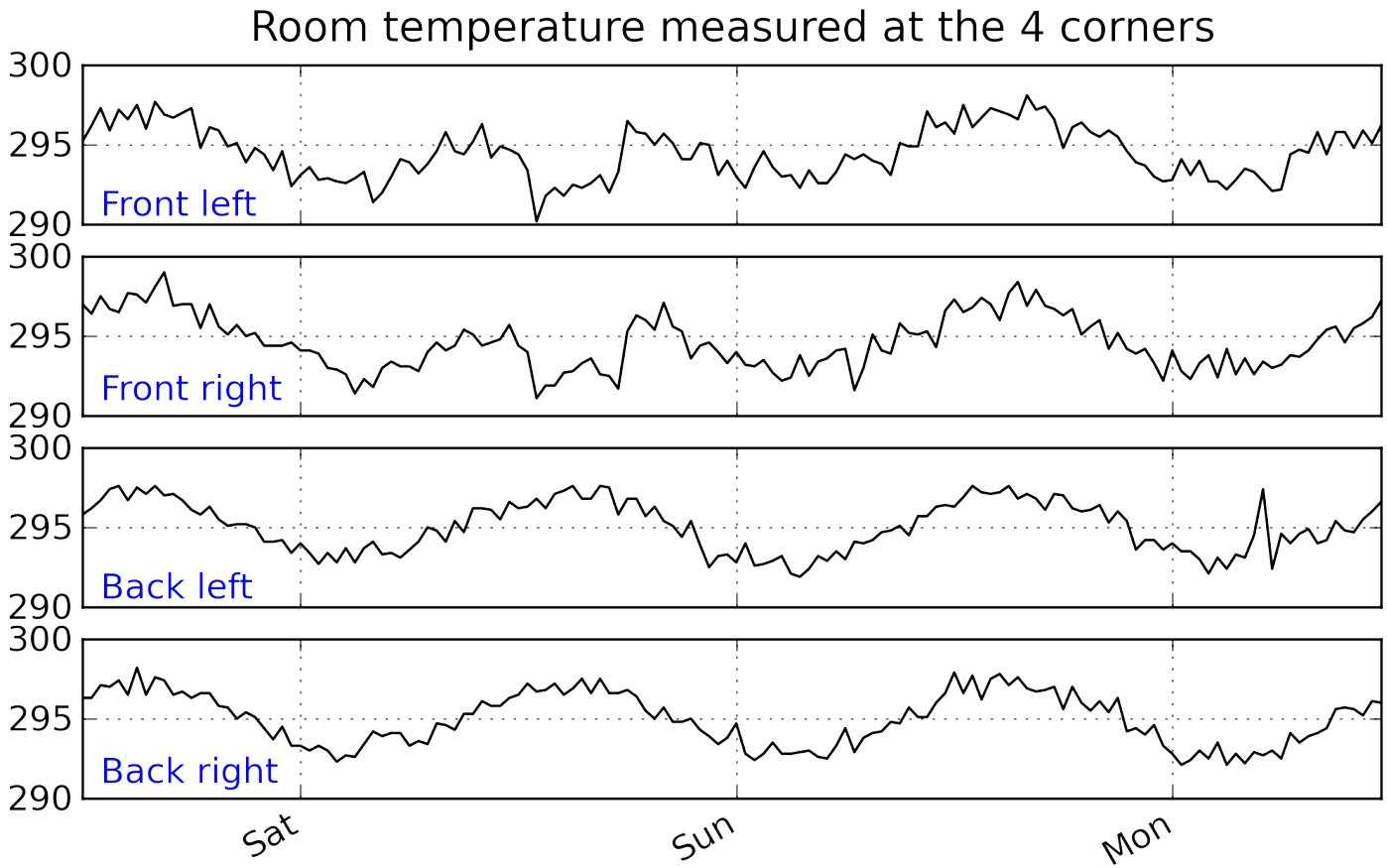
Your health

- No single measurement of "health"
  - blood pressure
  - cholesterol
  - weight
  - various length/circumference measurements
  - various ratios: BMI; waist/hip; etc
  - blood sugar
  - temperature, *etc*
- Combine these in some way? Trained doctor does this mentally.

Health is a latent (hidden) variable

What is a latent variable?

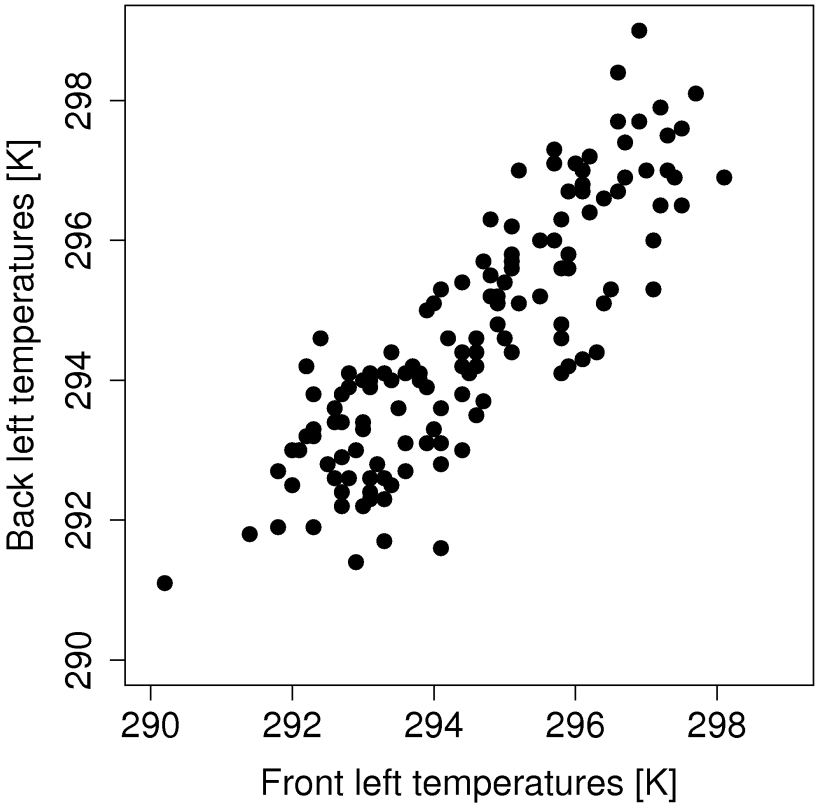
Temperature in this room

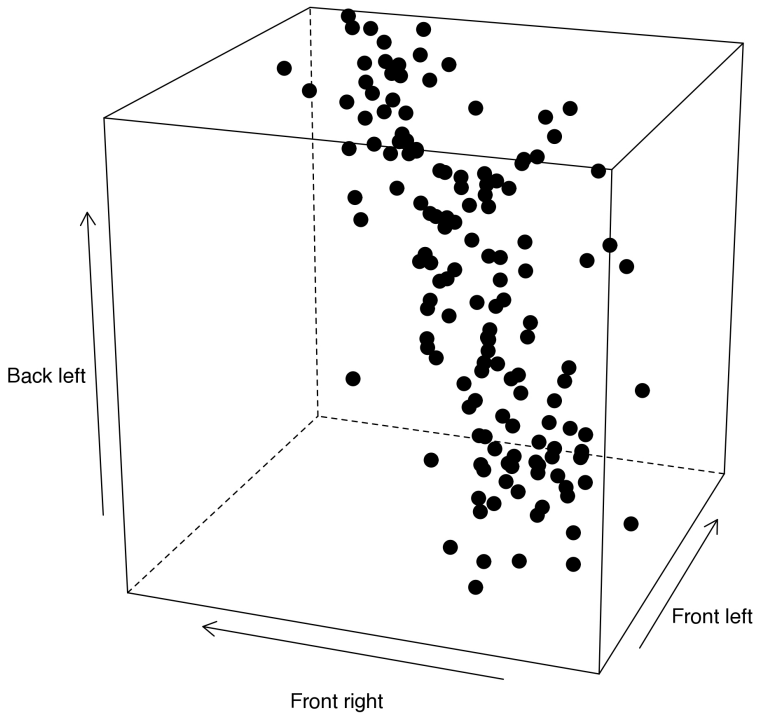


- What drives the movement up and down?
- Correlation of thermometers with the driving force.

What is a latent variable?

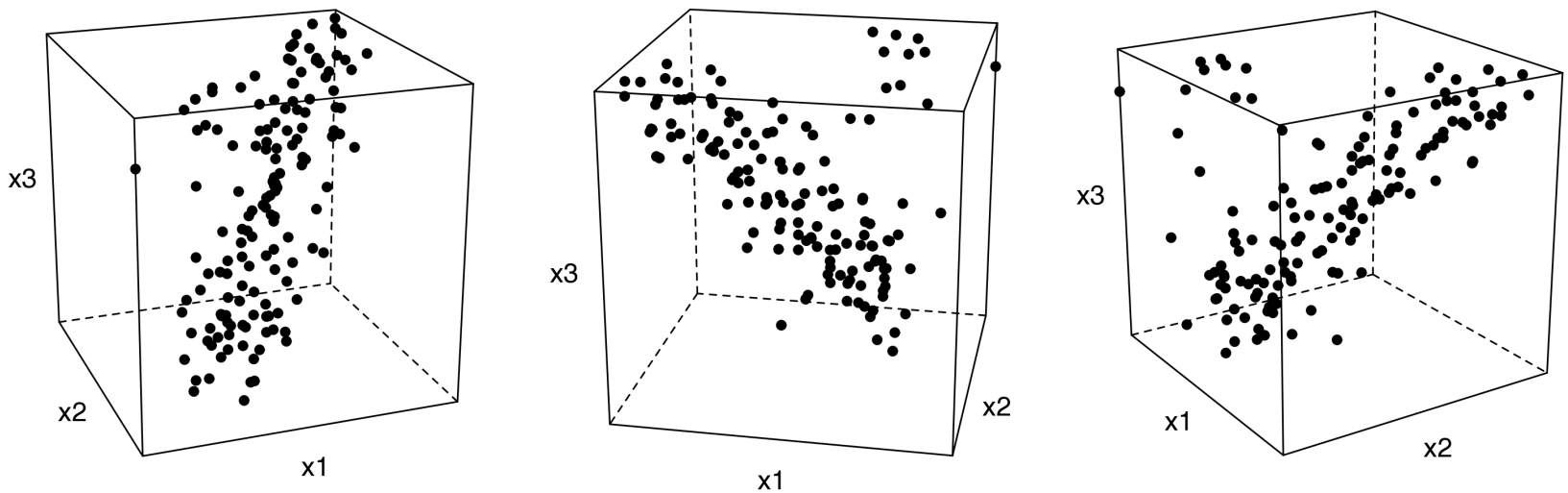
Temperature in this room: geometrically





- Each measurement in time is one point

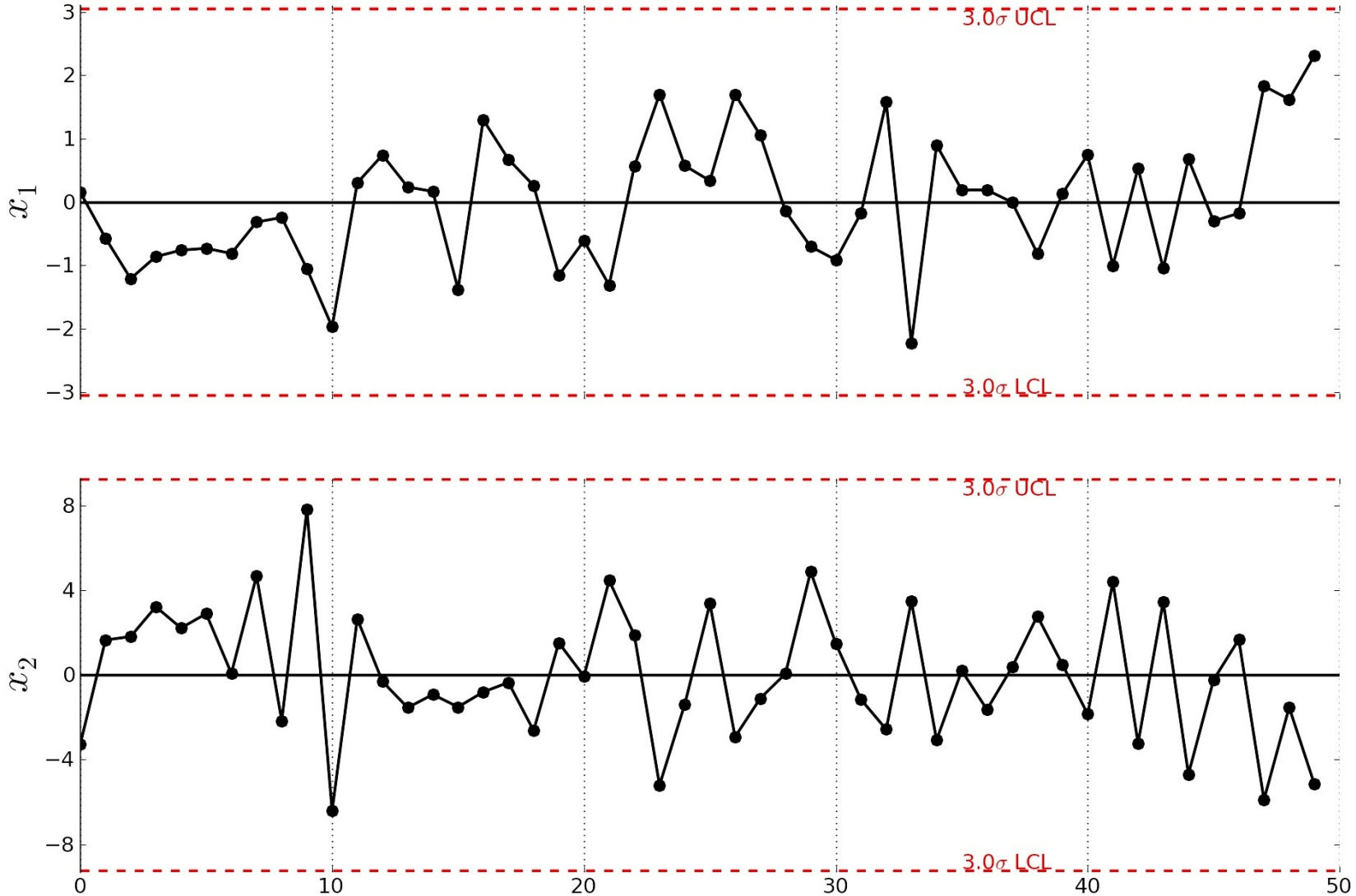
What is a latent variable?



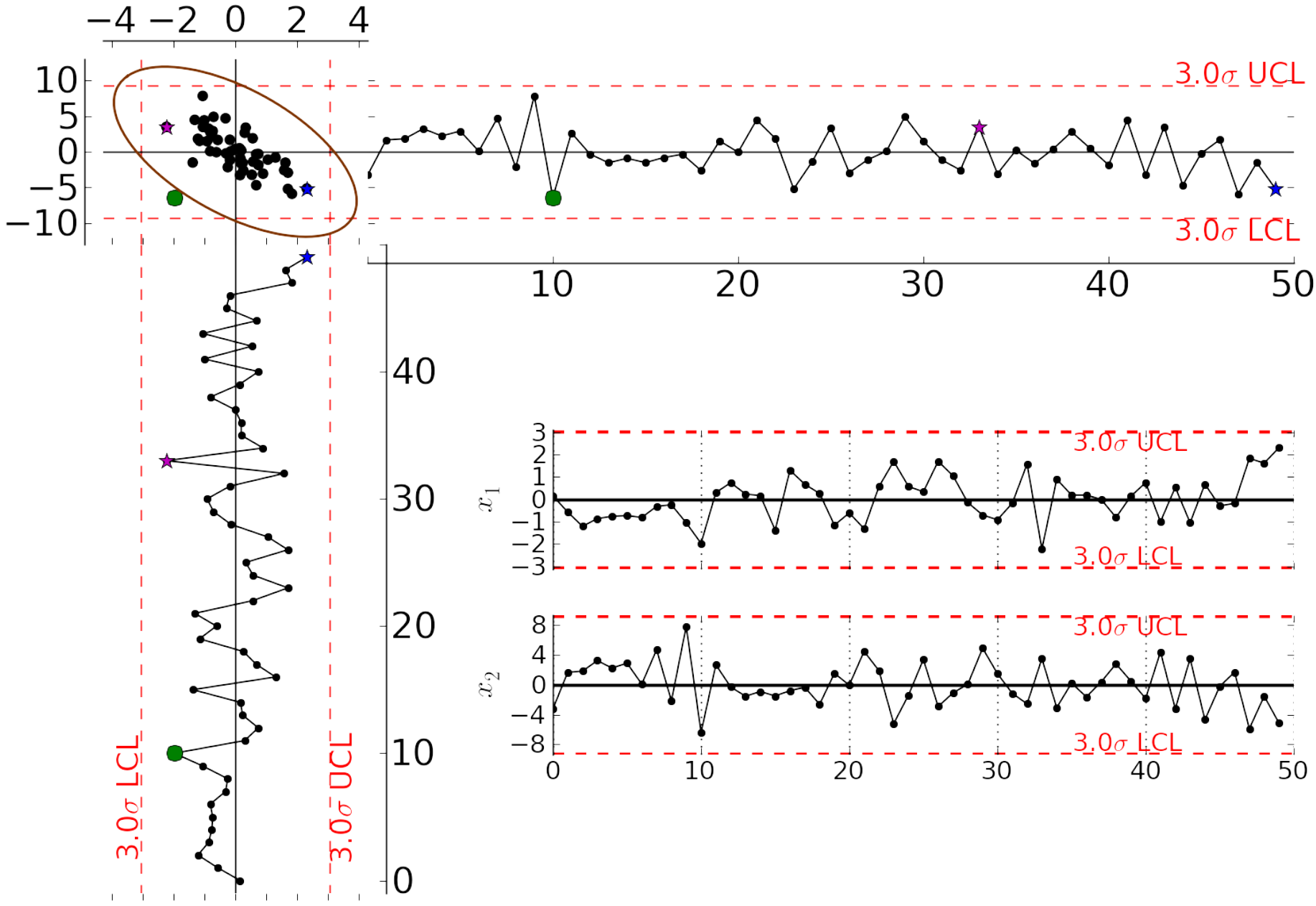
- Rotating plot demo

Why do we need latent variable methods?

- Shewhart chart for two variables, x_1 and x_2
  - e.g. final product quality from lab values

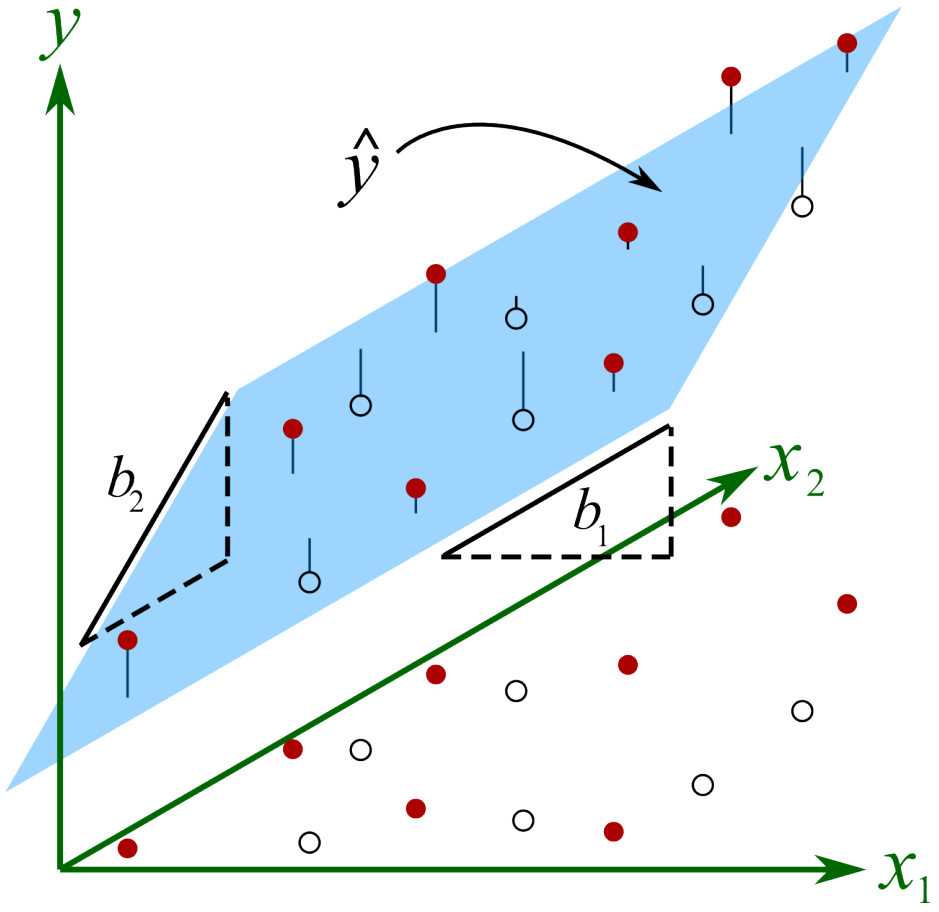


Why LVM? For process monitoring



LVM for regression

Multiple linear regression model: $y = b_1 x_1 + b_2 x_2$

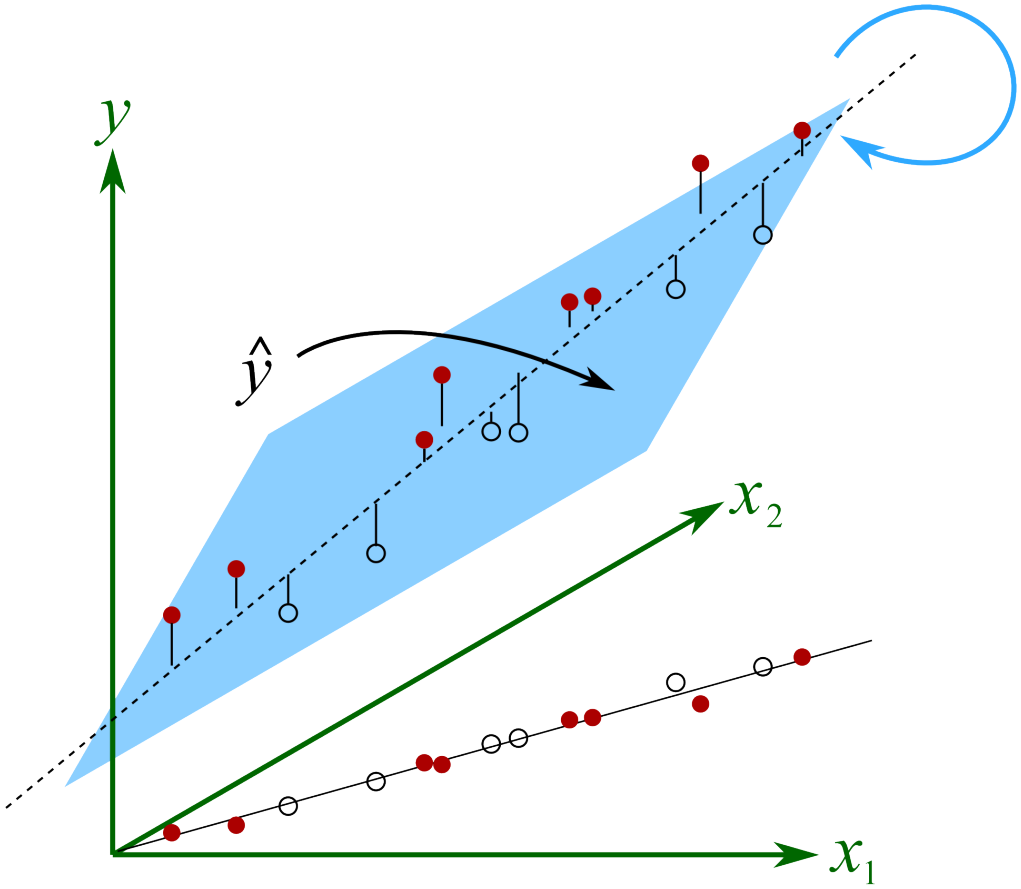


- Stable estimates are desirable:
  - for learning about the process
  - for accurate predictions in the future

- We get stable estimates for b_1 and b_2 when the plane is "well supported" by the measured points
- Think of DOE: we intentionally move to the corner points to fit the model

LVM for regression

- But what if the two x-variables are strongly correlated?



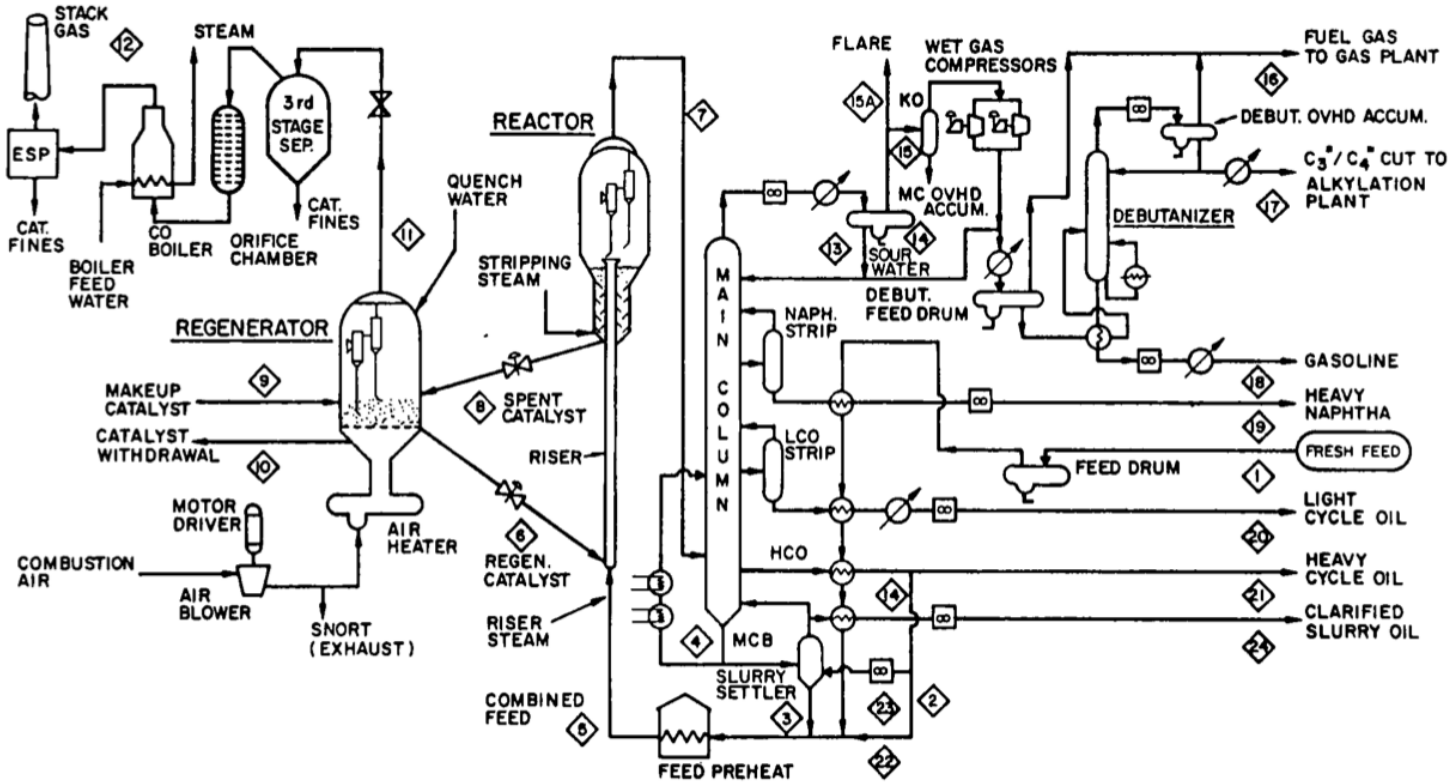
- The plane rotates for small changes in x-variables
- The slope coefficients change (can even change sign!)

LVM for regression

- What can I do about it?
- *Suboptimal solution*
  - Recognize that x_1 and x_2 are correlated
  - Choose either x_1 or x_2 in the model:
    - $y = b_0 + b_1 x_1$
    - $y = b_0 + b_2 x_2$
- Problems with correlated data
  - which variables do you choose to keep or throw out?
  - can I use an average of the two correlated variables?
  - how do you know what is "too strong correlation" before its problematic?
- Variable selection is not easy ....
  - Demo on a small example
- Solution: don't select variables !

LVM for troubleshooting

- ∼300 measurements
- 3.5 months of data
- How to uncover problems and visualize this much data?

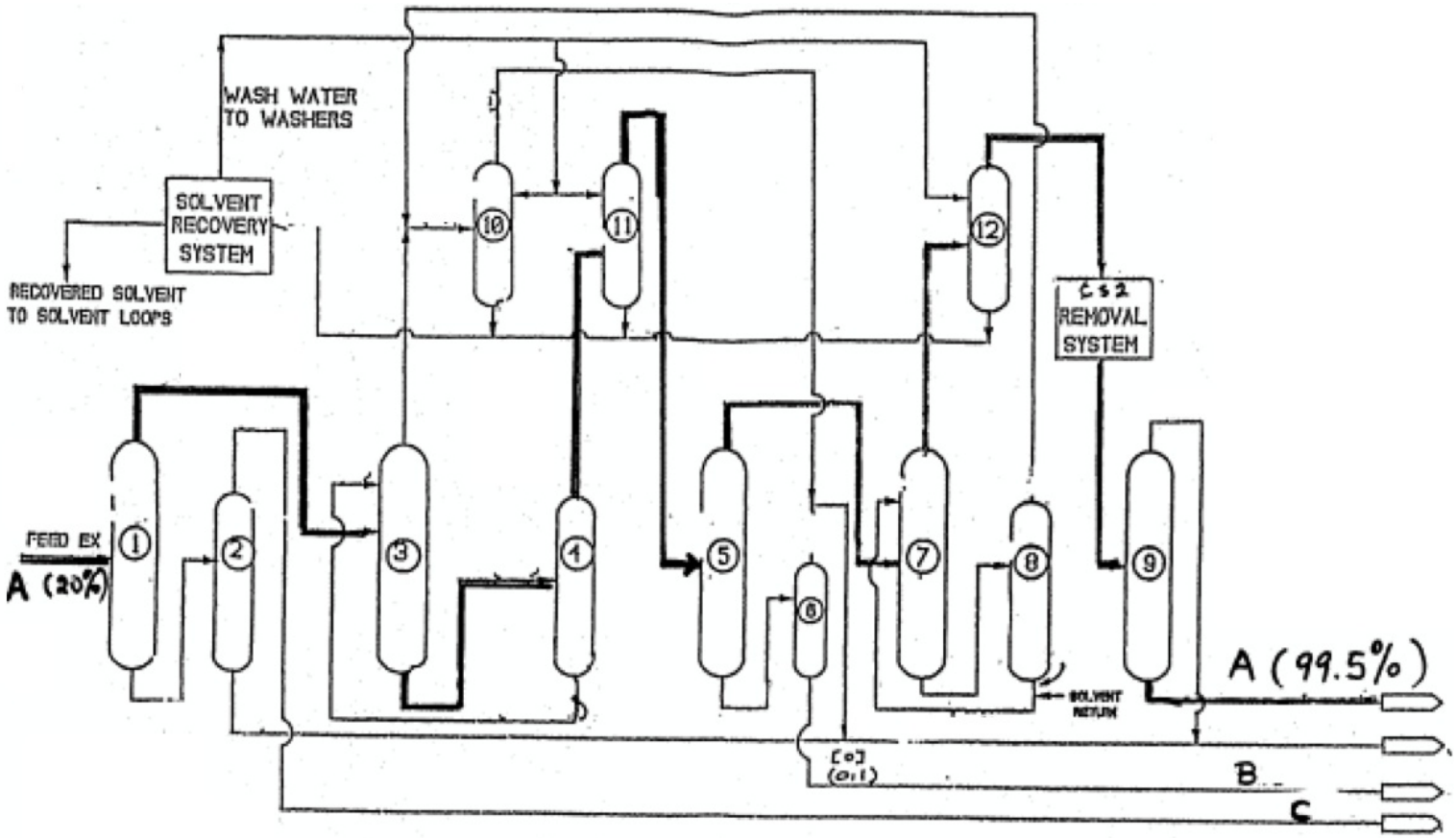


- *Carol Slama, Masters Thesis, McMaster University, 1991*
- http://digitalcommons.mcmaster.ca/opendissertations/3301

LVM for troubleshooting

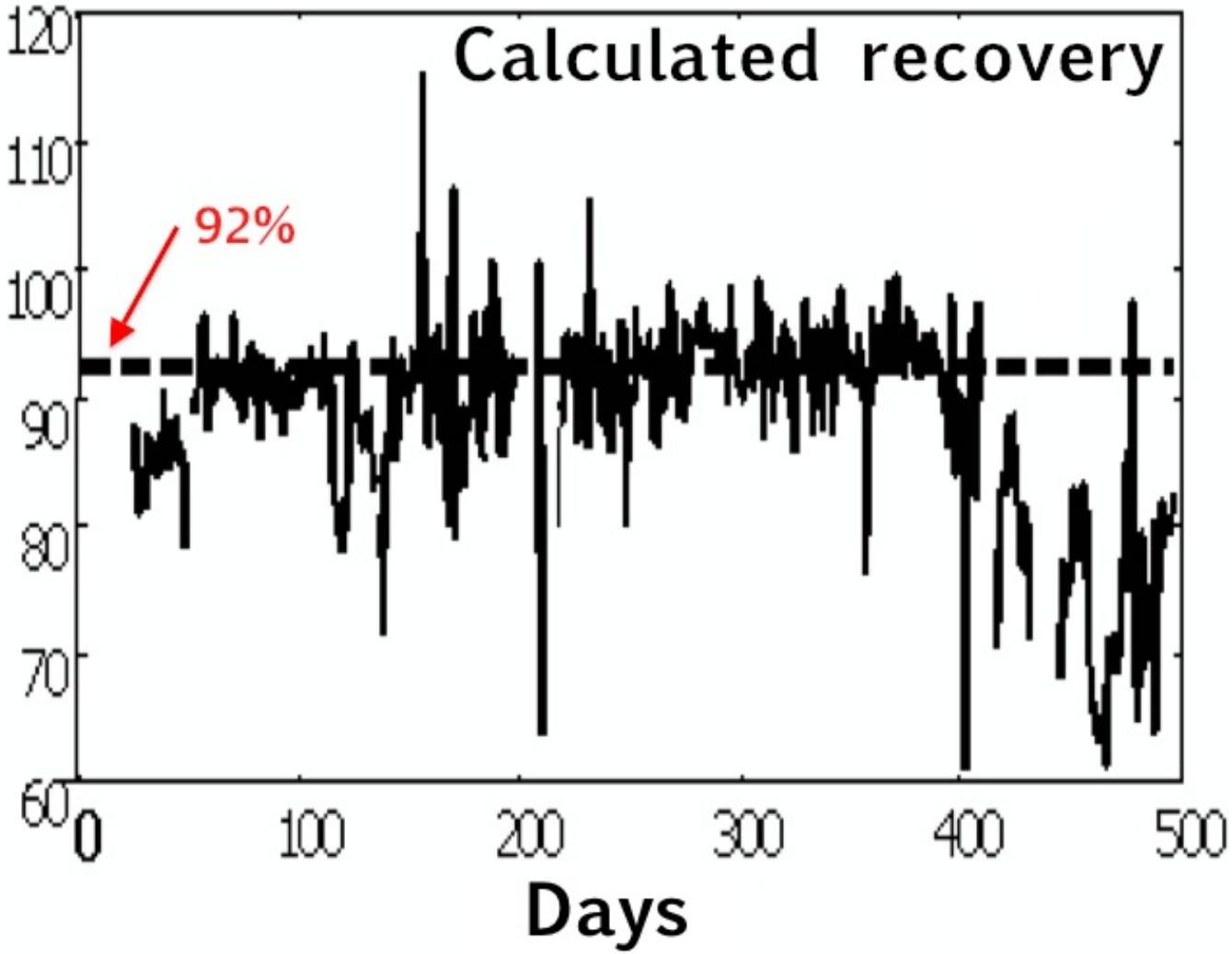
Monomer recovery flowsheet

- 447 tags measured (i.e. a 447 dimensional data cube)
- Data on about 500 days of operation



LVM for troubleshooting

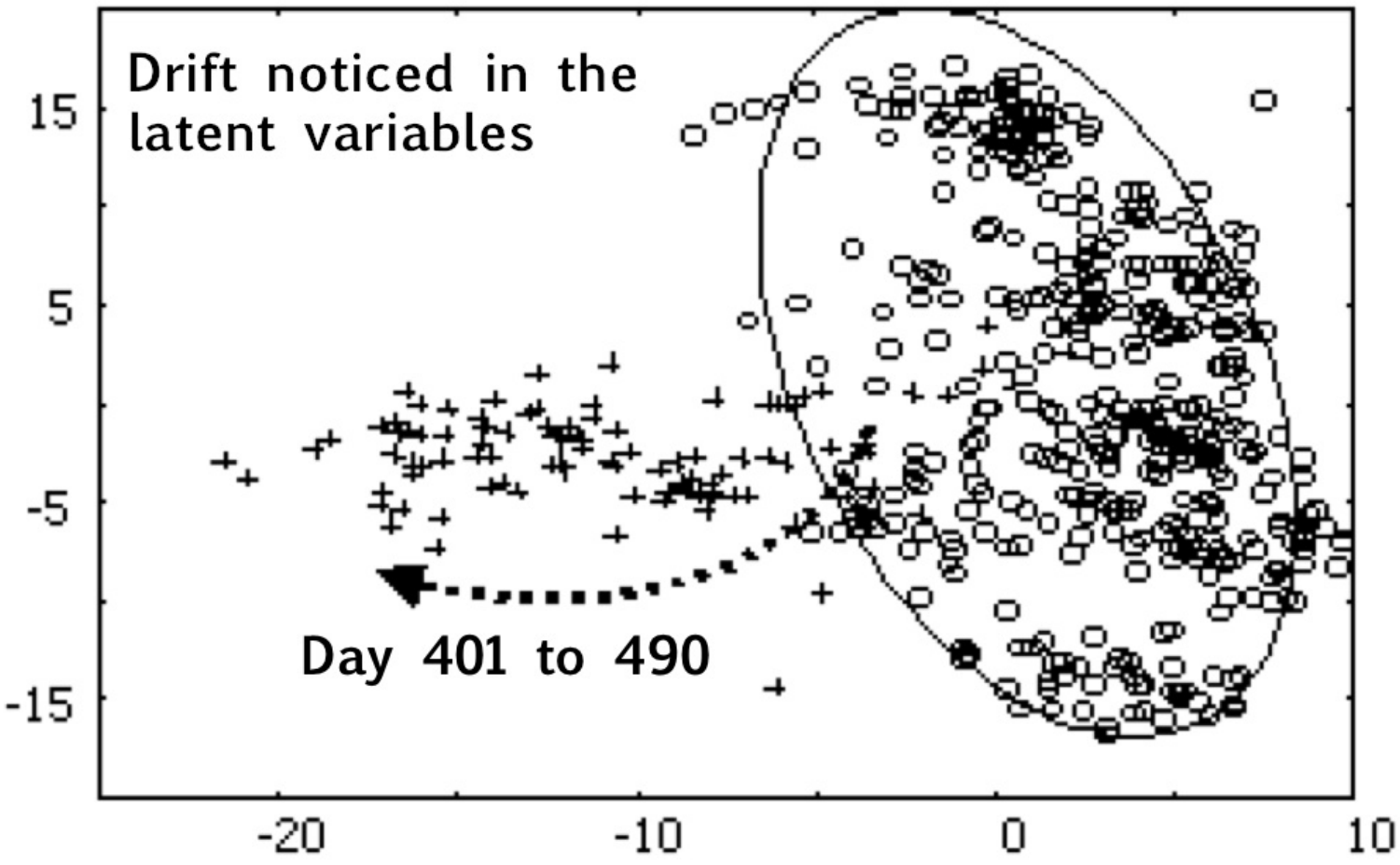
- Reduction in monomer recovery $\sim$ day 400. Target recovery $= 92\%$



- Engineers looked at various time series plots for several weeks
- 100 days elapsed without finding the cause

LVM for troubleshooting

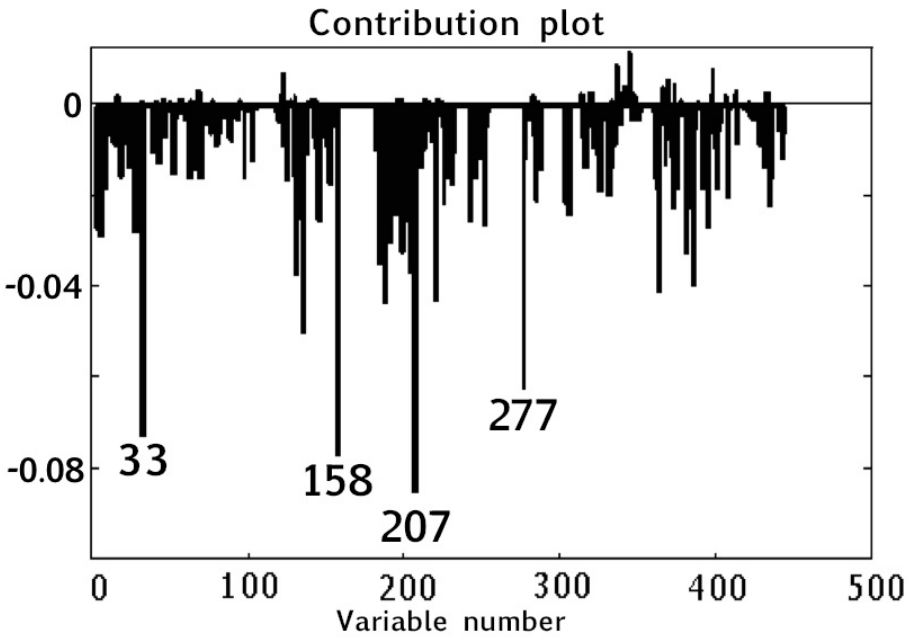
- A latent variable model with 2 variables was built
  - Compressed the 447 variables to 2 variables
  - Retains most of the information



- Interrogate the latent variables to see what changed ...

LVM for troubleshooting: contribution plot

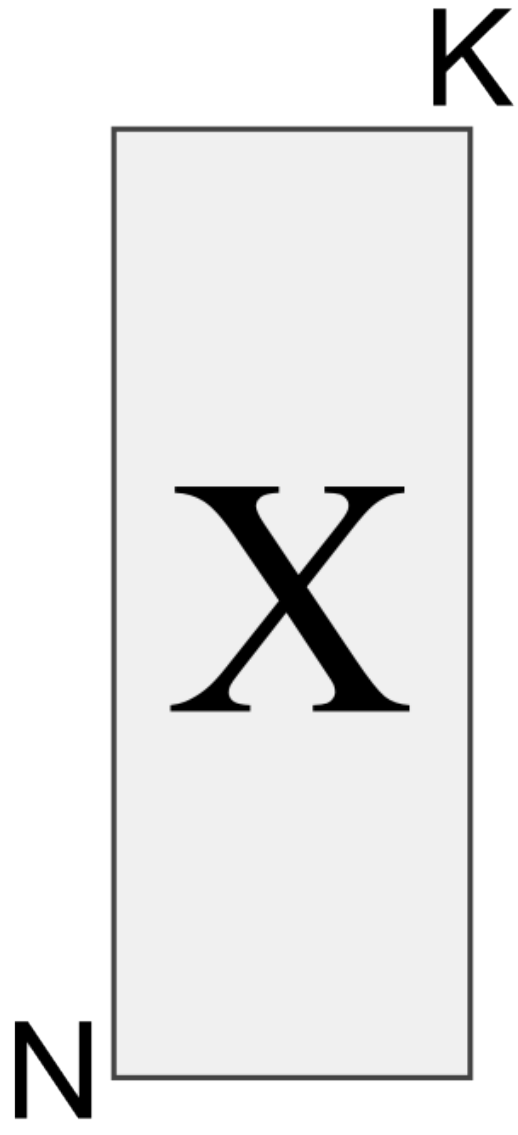
- Shows difference between two points in the score plot



- **207**: temperature on tray 129 in distillation column #3
- **158**: a tag from distillation column #3
- **33** and **277**: related to concentration of feed A

- *Suggests*: bad temperature control on tray 129 when feed concentration is high
- Fixed the controller and recovery went back to normal

Types of data we deal with

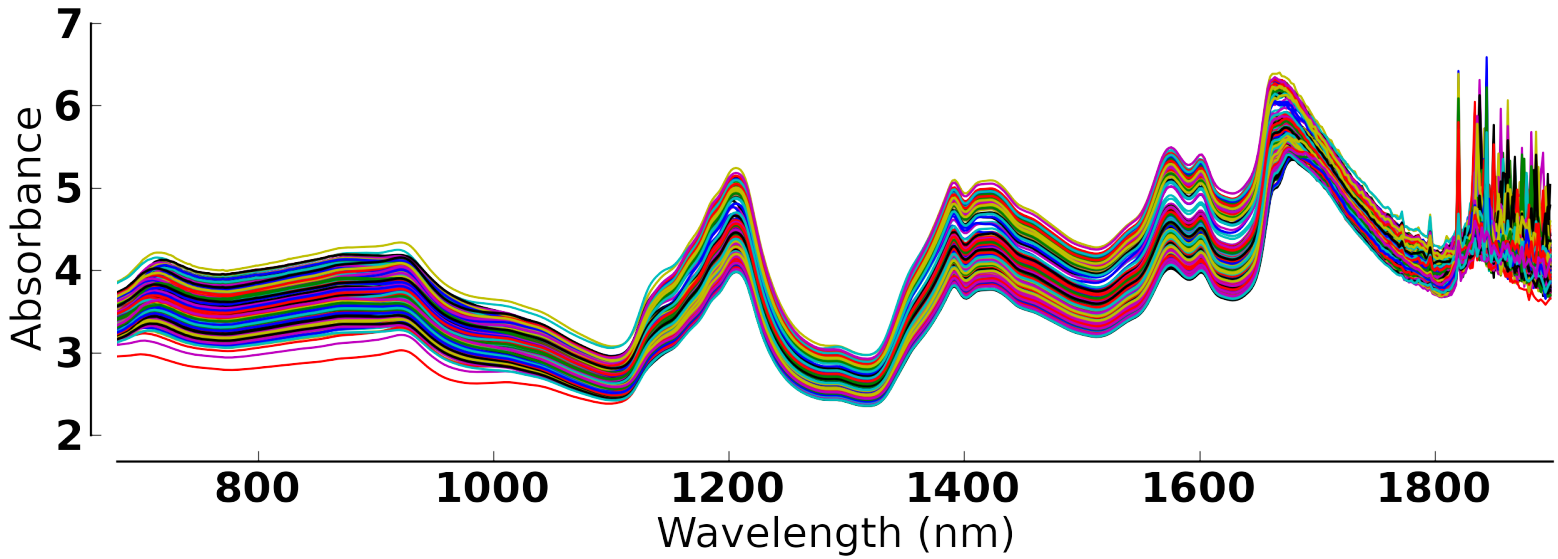


1920's to 1950's:

- small number of columns
- scatter plots
- time-series plots for each column
- Shewhart and EWMA charts
- multiple linear regression (MLR)
- carefully chose which columns to measure
  - independent
  - low error

Types of data we deal with

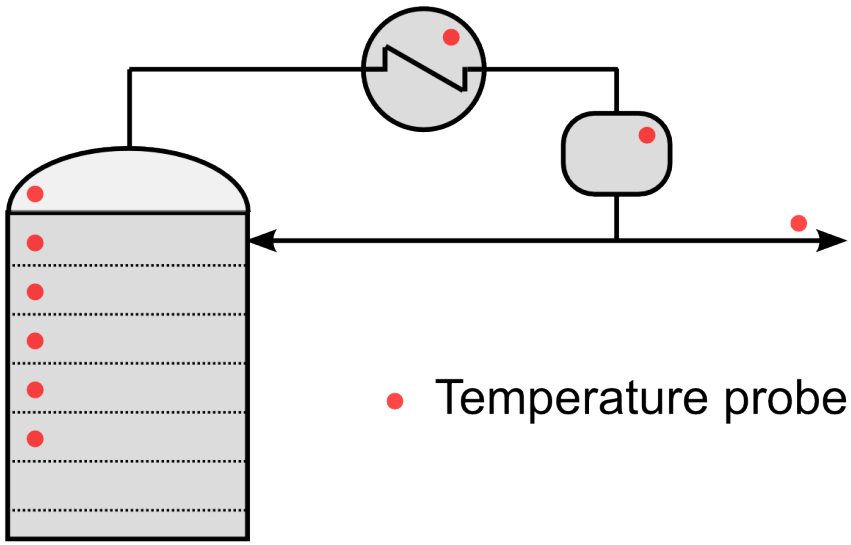
- **Small N and small K**
  - expensive measurement, low frequency
  - use scatterplots, linear regression, *etc.*
- **Small N and large K**



- Cannot use MLR directly: $K > N$

Types of data we deal with

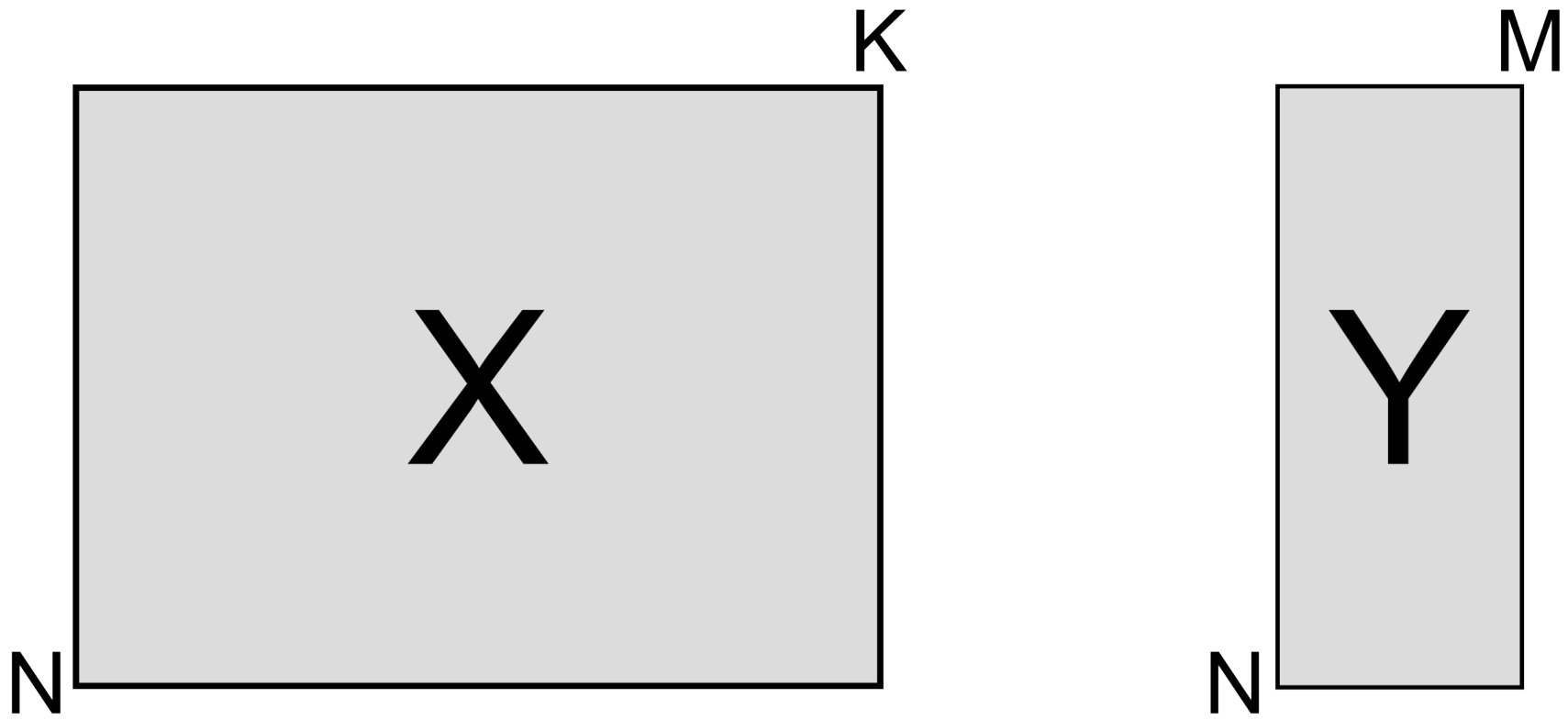
- **Large N and small K**
  - Refinery, most chemical plants
  - 2000 to 5000 variables (called tags) every second
  - 50 to 100 Mb per second



35 temperatures, 5 to 10 flow rates, 10 pressures, 5 derived values

Types of data we deal with

- **X and Y matrices**

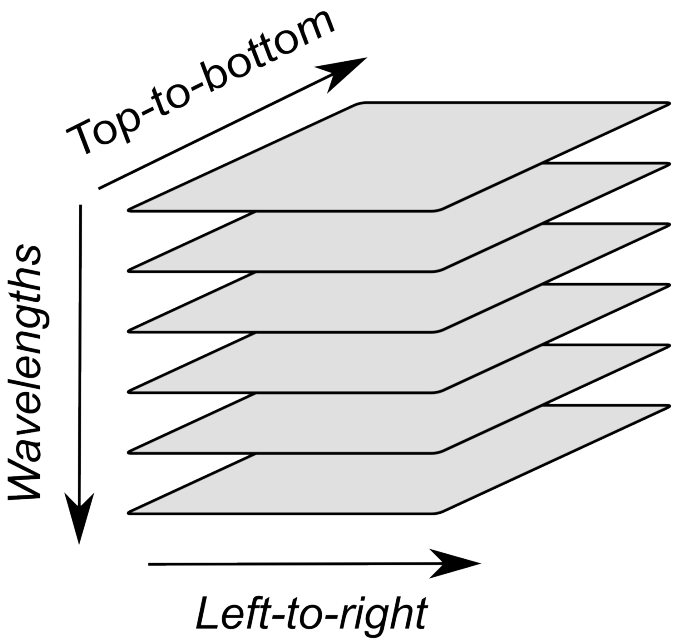


- Predict one or more variables
- Could use MLR; fails for highly correlated data

Types of data we deal with

- **3D data sets and higher dimensions**

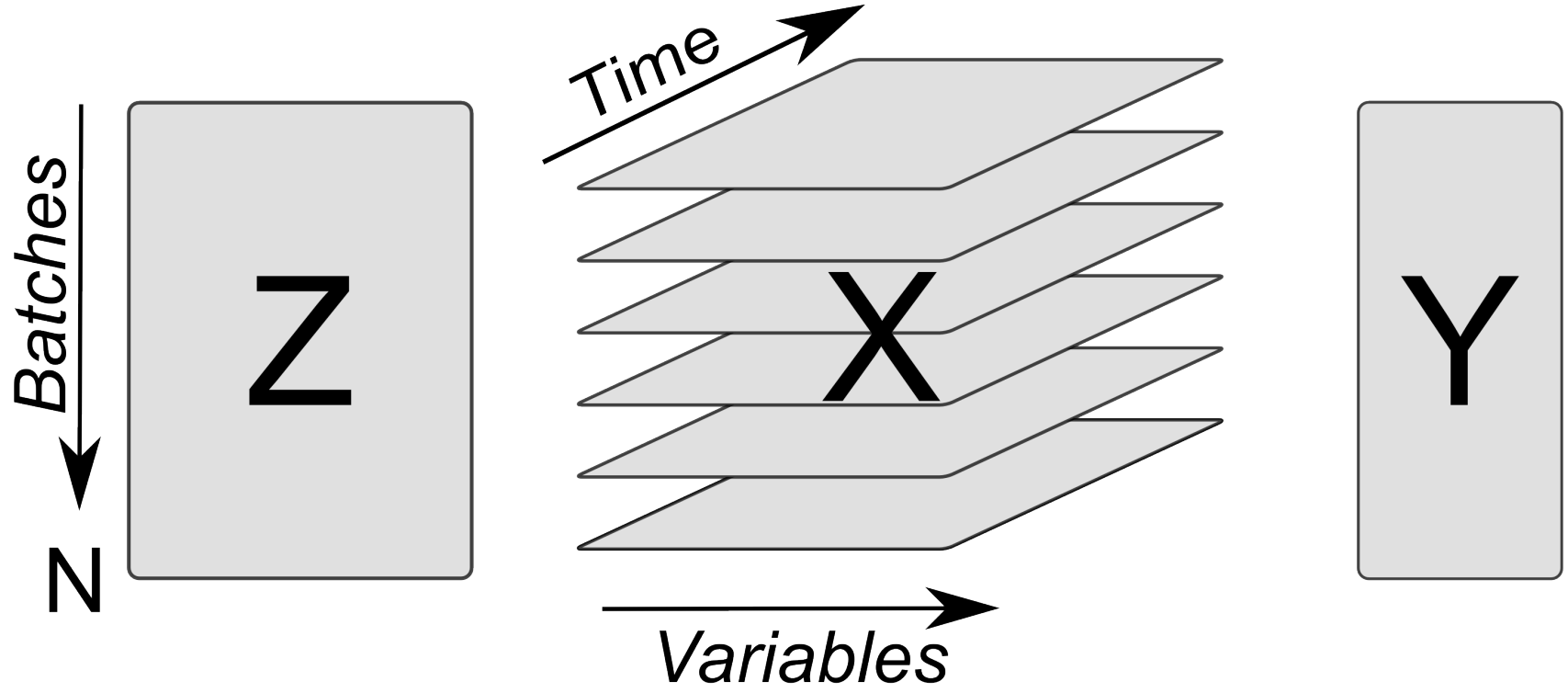
- Very common situation now
- Image data (medical imaging)



- 4th dimension: time
- Very high redundancy: neighbouring pixels are similar (spatially and in time)

Types of data we deal with

- **Batch data sets**



Issues faced with engineering data

- **Size of the data**
  - rows: we can deal with this
  - columns: $K(K-1)/2$ pairs of scatterplots
- **Lack of independence**
  - $\mathbf{X}^T\mathbf{X}$ becomes singular
  - make-shift approach: pick a reduced set of columns
- **Low signal to noise ratio**
  - aim to keep our processes constant
  - little signal and high noise
  - data collected is mostly uninformative: constant, noisy, has drift and error
  - Called "happenstance data"

Issues faced with engineering data

Non-causal data

- Happenstance data is non-causal
  - Only see correlation effects
  - Good enough in many cases
- Opposite case: a designed experiment
  - cause-and-effect

Issues faced with engineering data

- **Errors in the data**
  - Least squares: assumes no error in X
  - Not realistic in most cases
- **Missing data**

	A	B	C	D	E	F	G	H	I	J	K	L	M
1		Ton_in	KR30_IN	KR40_IN	PARM	HS_1	TOTAVF	PAR	FAR	r_FAR	%Fe_FAR	%P_FAR	%Fe_malm
2	1	0	0	4.65	1.6	84.9314	5.275	25	0.0625	0.249377			
3	2	0	0	4.65	1.25	84.9314	4.775	10.75	0.0625	0.578035			
4	3	0	0	0	6.95	84.9314	-3.5125	7.8125	0.0625	0.793651			
5	4	0	0	0	0.2	84.9314	3.2375		0.0625	100			
6	5	0	0	0	1.4625	84.9314	1.975		0.0625	100			
7	6	0	0	0	4.1	89.6072	-0.6625	7.3125	0.0625	0.847458			
8	7	0	0	0	1.05	89.236	2.375	6.75	0.0625	0.917431			
9	8	0	0	0	1.4	89.926	2.025	6.3125	0.0625	0.980392			
10	9	0	0	0		90.2119	3.225	6.5	0.0625	0.952381			
11	10	0	0	0		90.3292	3.0125	5.75	0.0625	1.07527			
12	11	1271.81	275.813	190.875	62.975	90.4108	383.706	307.875	591.75	65.7774	66.2	0.24	47.9
13	12	1290.56	278.55	208.575	58.075	90.4108	384.281	314.625	601.5	65.657	66.2	0.24	47.9
14	13	1267.39	278.55	207.375	63.1875	90.4108	398.212	312.188	585.063	65.2062	66.2	0.24	47.9
15	14	1250.44	278.063	204.525	57.475	90.4108	384.556	298.625	576.75	65.886	66.2	0.24	47.9
16	15	1265.51	279.563	190.425	49.3125	90.4108	415.381	304.125	591.75	66.0527	66.2	0.24	47.9
17	16	1268.18	276.112	194.625	62.875	90.4108	403.706	310.875	592	65.5683	66.2	0.24	47.9
18	17	1284.3	272.55	211.275	58.675	90.4108	405.331	293.125	575.5	66.2541	66.2	0.24	47.9
19	18	1284.41	275.4	208.275	50.475	90.4108	420.531	304.125	580	65.6016	66.2	0.24	47.9
20	19	1272.79	274.35	207.525	62.675	90.4108	394.569	300.125	598.25	66.5925	66.2	0.24	47.9
21	20	1317.11	269.813	192.225	56.175	90.4108	409.681	311.125	579.75	65.0765	66.2	0.24	47.9
22	21	1273.16	264.712	195.375	49.5625	90.4108	405.469	291.625	585.25	66.7427	66.2	0.24	47.9
23	22	1048.39	213.113	166.538	32.5125	94.5204	339.569	248.563	491.688	66.4218			
24	23	1019.66	217.875	192.525	31.4125	94.5204	330.044	264.625	494.438	65.1379			
25	24	1049.06	222.375	183.525	35.7125	94.5204		258.875	479.438	64.9369			
26	25	1057.5	215.625	177.825	33.275	94.5204		238.125	535.25	69.2096			
27	26	1036.95	211.125	165.375	26.2125	94.5204		244.313	490.438	66.7489			
28	27	1057.95	218.025	168.488	35.2625	94.5204		237.063	485.938	67.2113			
29	28	1033.05	212.512	179.475	33.4125	94.5204		254.625	520.5	67.1505			
30	29	1041.38	212.475	170.738	24.5	94.5204		256.375	507.75	66.4485			
31	30	1062.49	217.613	170.625	32.4125	94.5204		242.563	477.188	66.2991	67.2	0.2	51.2
32	31	1024.8	218.063	178.425	43.4625	94.5204		261.125	505.5	65.9384	67.2	0.2	51.2
33	32	1070.74	215.063	165.337	38.5125	94.5204		248.563	501.75	66.8721	67.2	0.2	51.2
34	33	1054.65	216.075	176.025	31.4125	94.5204		249.563	523	67.6968	67.2	0.2	51.2
35	34	1072.05	214.725	166.238	41.075	94.5204		263.563	514.5	66.1258	67.2	0.2	51.2
36	35	1056.71	224.625	177.675	35.3125	94.5204		252.875	522.25	67.3762	67.2	0.2	51.2
37	36	1018.13	223.275	161.587	12.4	94.5204	250.225	222.125	577.563	72.2235			

Issues faced with engineering data

Tools that we require:

- extract relevant **information** from data
- deal with missing data
- 3-D, 4-D and higher data sets
- combine data from different sources (same object)
- handle collinearity (low signal to noise ratio)
- handle error in recorded data

Latent variable methods are a suitable tool that meet these requirements.

Examples of interesting data sets: Millau Viaduct

In France: expressway connecting Paris and Barcelona

Examples of interesting data sets: Millau Viaduct

Examples of interesting data sets: Millau Viaduct

Examples of interesting data sets: Millau Viaduct

- Pylons, deck, masts have anemometers, accelerometers, inclinometers, extensometers, and temperature sensors
- Detect movement (micrometer level), monitor for oscillations, stress/strain
- Piezoelectric sensors gather traffic data: weight, speed, density of traffic
- Can distinguish between fourteen different types of vehicle
- 100 readings per second from the main pylon
- Data transmitted via ethernet and fibre optic cables

Other data sources

- Chemical plants are moving to wireless sensors and networks
- More and more data available **and accessible** to engineers than even before
  - Prior to about 2005: data recorded, but not easily available

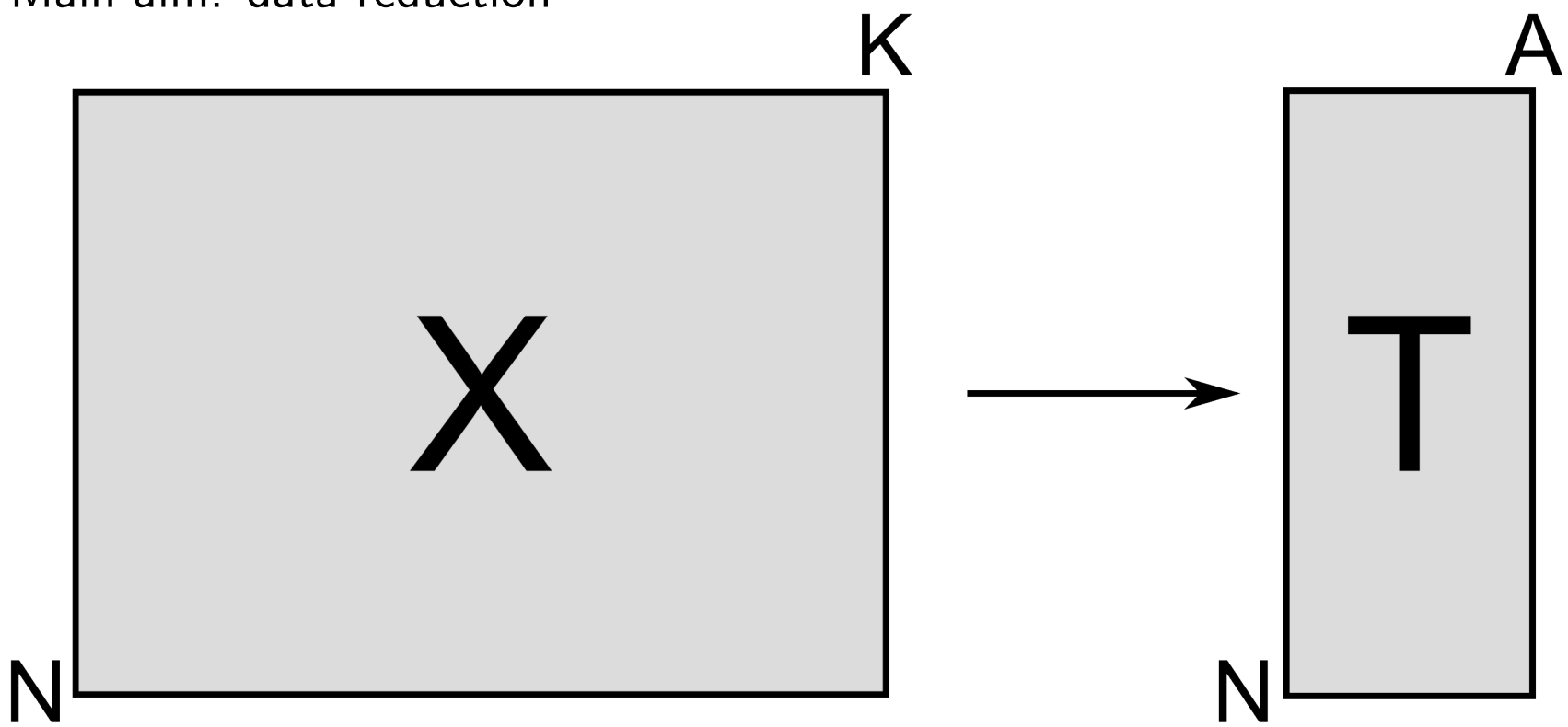
The "large data set" trap

It's not about the size of your data ... it's what you do with it.

- Many **rows**?
  - use a for loop
  - use parallel computing
  - Amazon EC2:
    - Simple CPU rent: \$0.17/hour
    - 23 GB memory, 4-core CPU, 1.7 TB storage, 64-bit: \$1.60/hour
- Many **columns**?
  - are they really all independent?
  - use latent variable methods

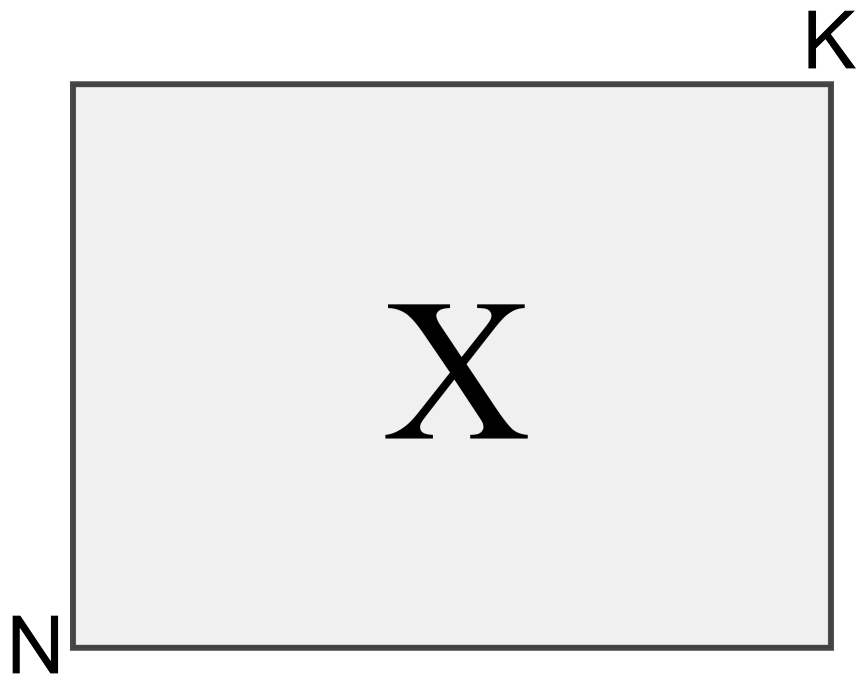
Principal component analysis (PCA)

Main aim: data reduction



Principal component analysis (PCA)

- PCA considers a single matrix: $\mathbf{X}$



- N observations
- K variables
- What goes in $\mathbf{X}$?
  - Any variable we measure
  - Calculations about the process
  - Theoretical knowledge: e.g. dimensionless numbers

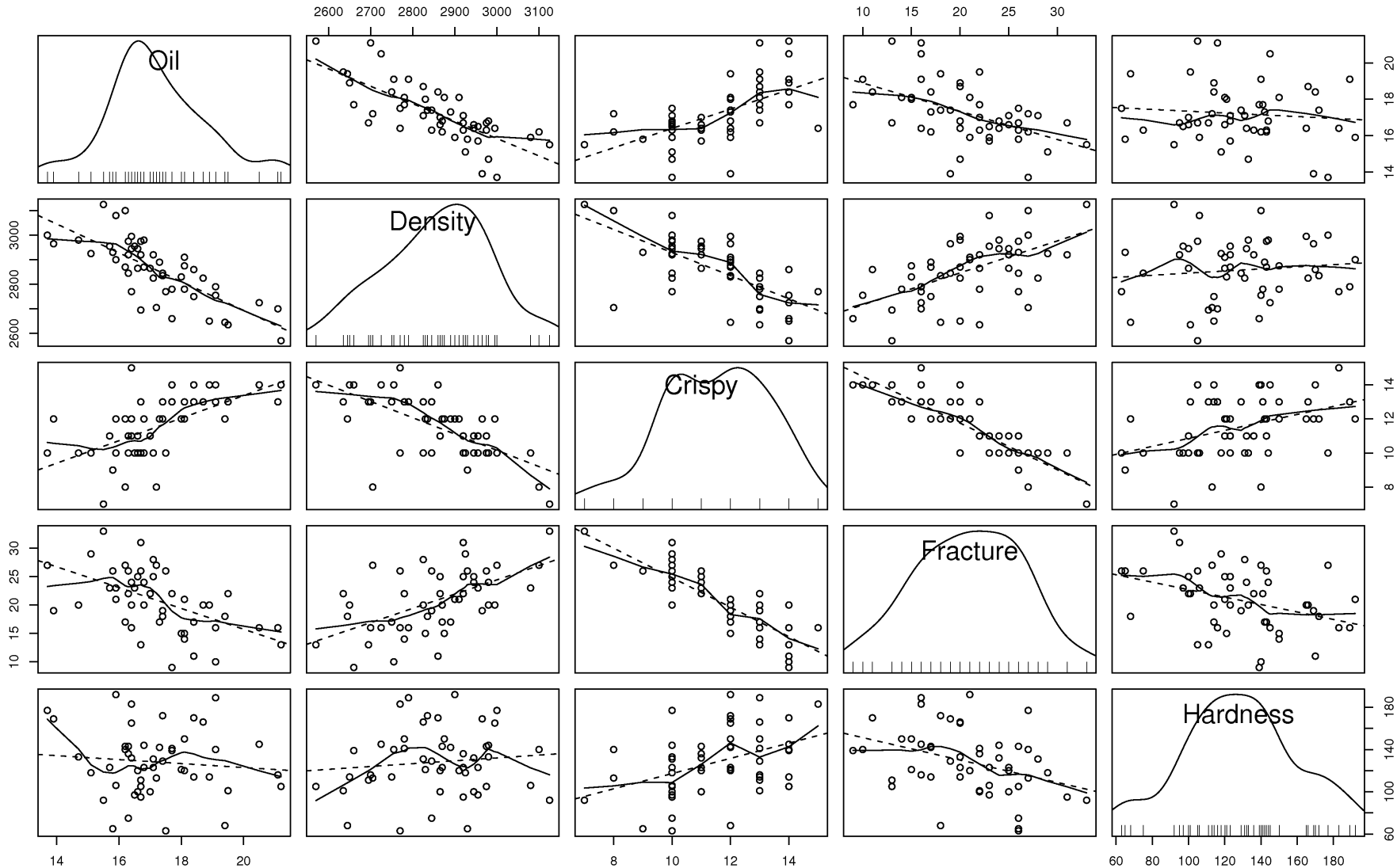
Food texture example

5 quality attributes are measured from pastries:

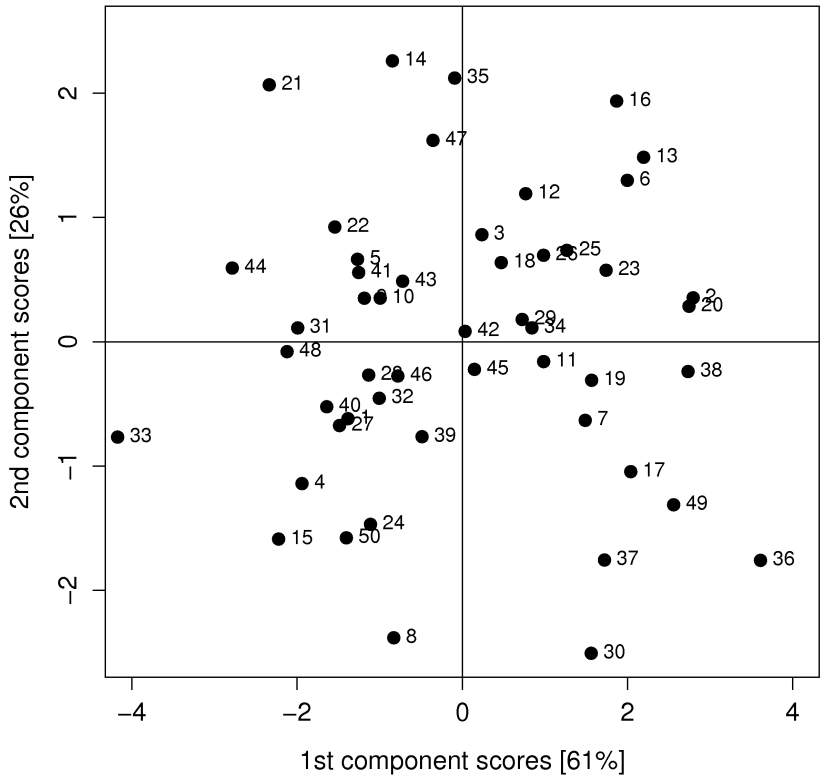
1. Percentage oil
2. Density
3. Crispiness measurement: from 7 (soft) to 15 (crispy)
4. Fracture angle
5. Hardness: force required before it breaks

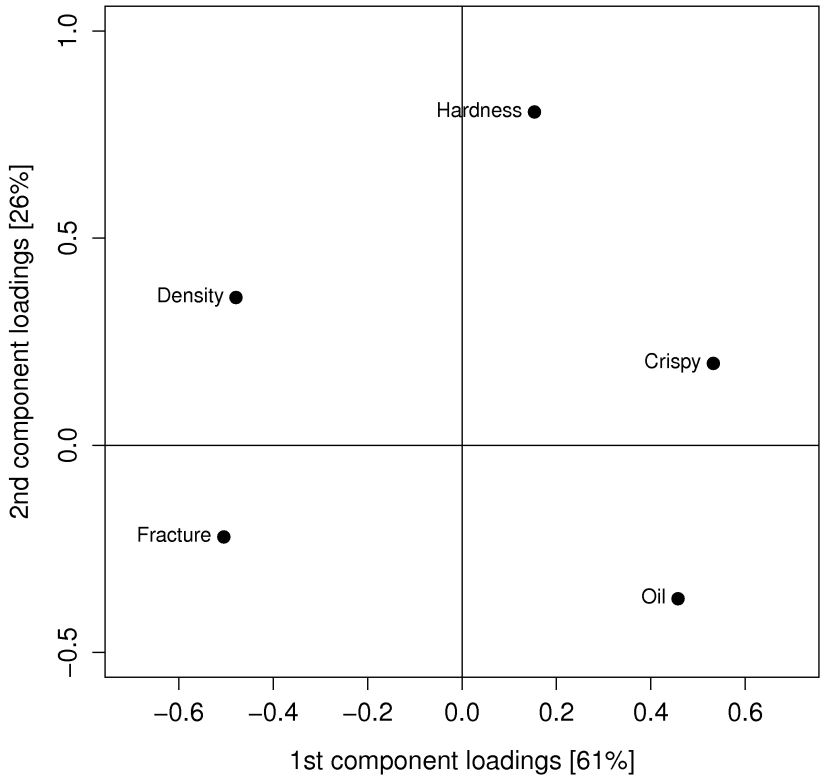
- 54 measurements on these 5 variables
  - How to visualize?
  - Scatter plot matrix (good when $K < 10$)

Food texture example



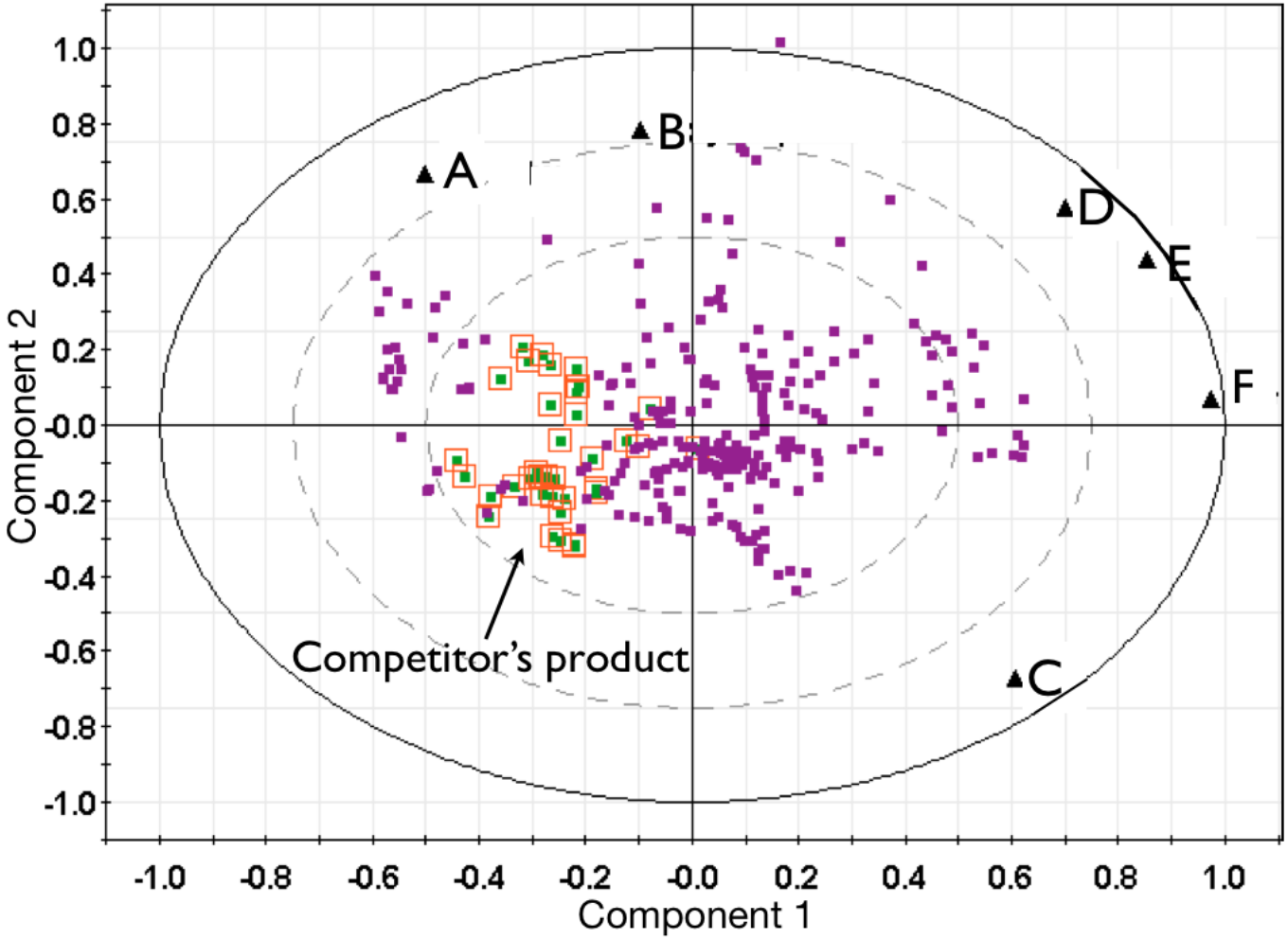
Food texture example: PCA model





- 87% of variance of 5 variables captured with 2 variables (13
- We cannot independently move the 5 quality variables

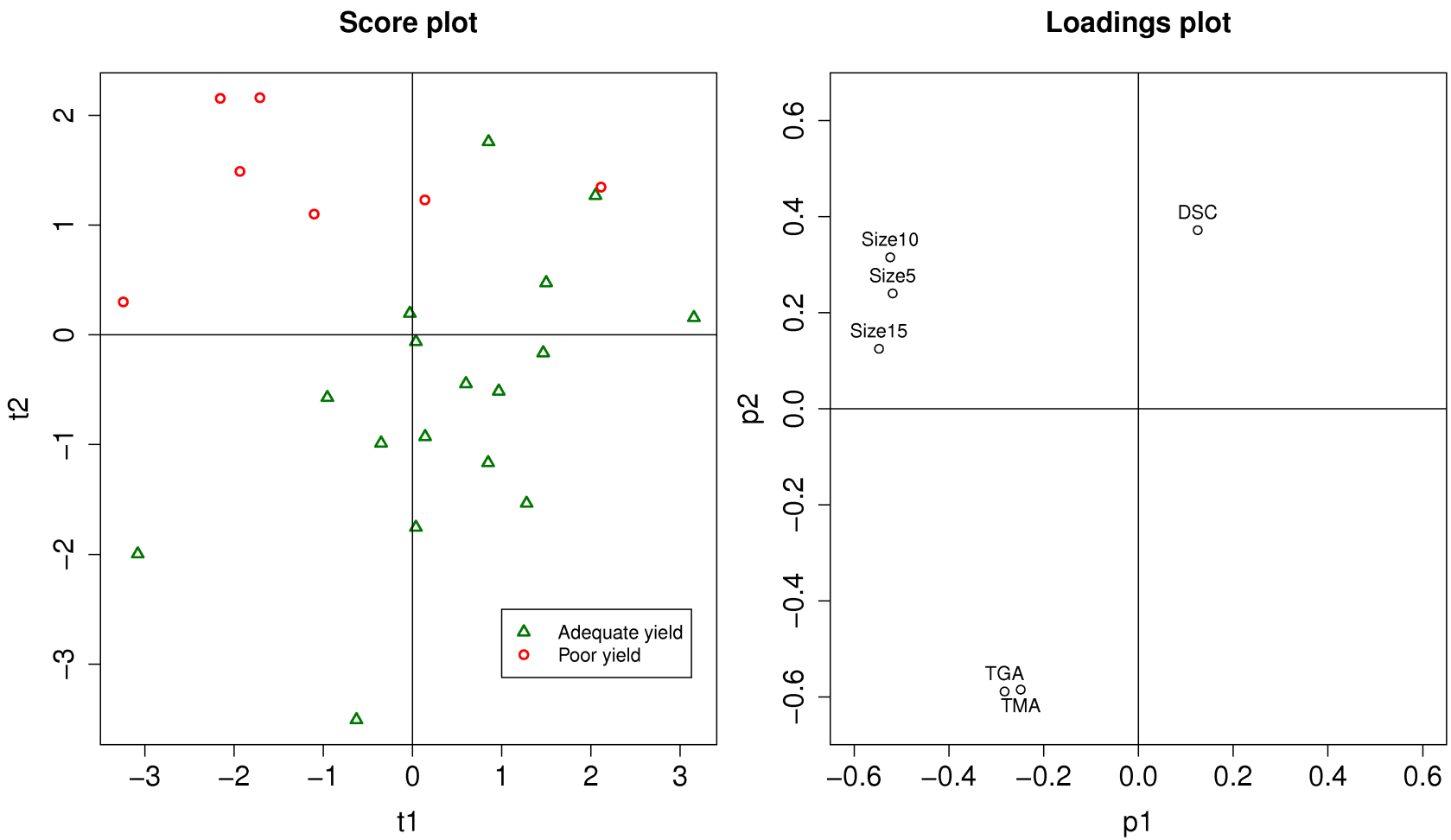
Improved process understanding



- Learn which variables are correlated
- Competitor has much less variability !
- Can we reproduce the competitor's product? *Yes*

Troubleshooting process problems

- Yield was declining
- 6 measurements: 3 size-related, 3 from the lab



Process monitoring

Monitoring with latent variables:

- We have K variables (tags)
- Reduce this to A scores (latent variables)
- Combine these A scores to a single value: Hotelling's T^2
- Errors: combined into a single value: SPE

Advantages:

- The scores are orthogonal
- Fewer scores than original variables
- Monitor anywhere that there is real-time data
- Don't have to wait for the lab's final measurement

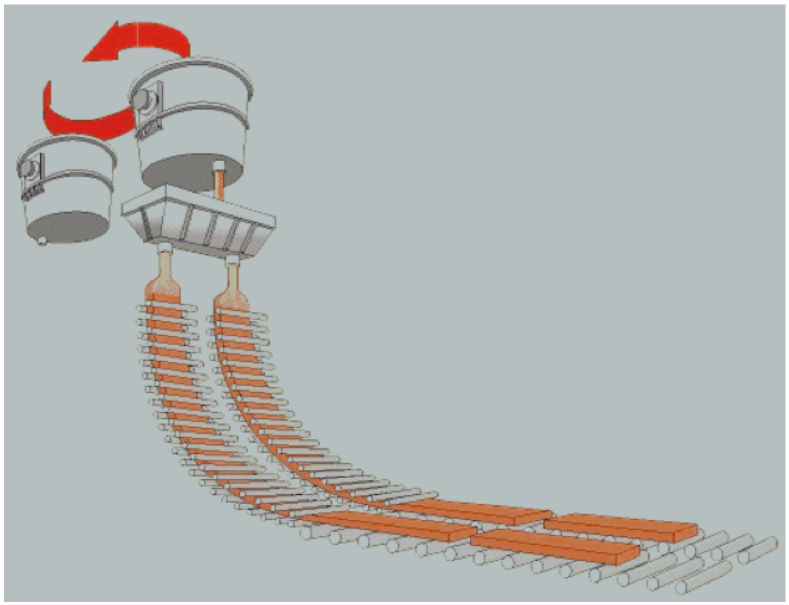
Industrial case study: Dofasco

- ArcelorMittal in Hamilton (formerly called Dofasco) has used multivariate process monitoring tools since 1990's
- Over 80 latent variable applications used daily
- Most well known is their casting monitoring application, Caster SOS (Stable Operation Supervisor)
- It is a multivariate monitoring system

Dofasco case study: slabs of steel

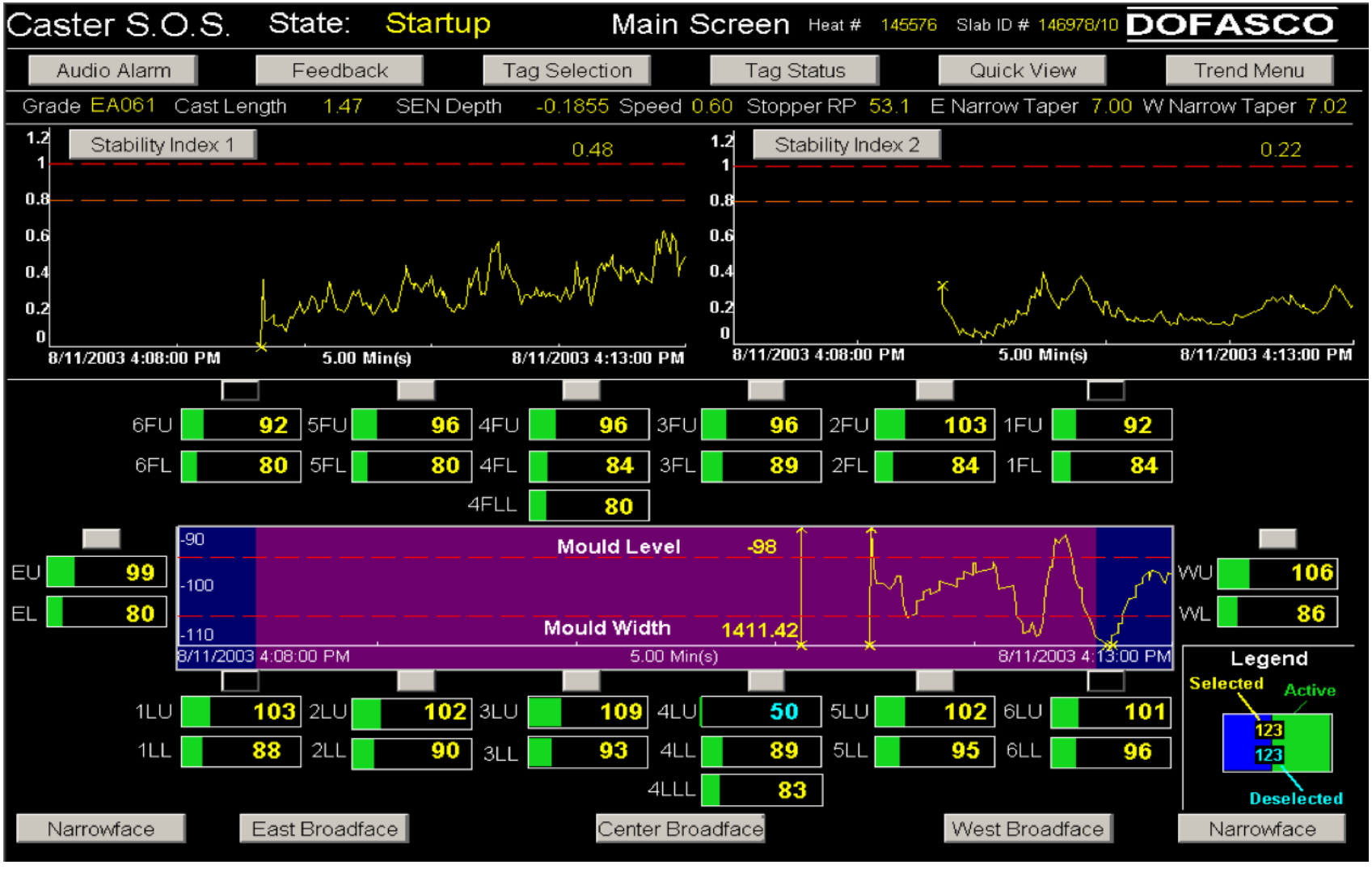
All screenshots with permission of Dr. John MacGregor

Dofasco case study: casting

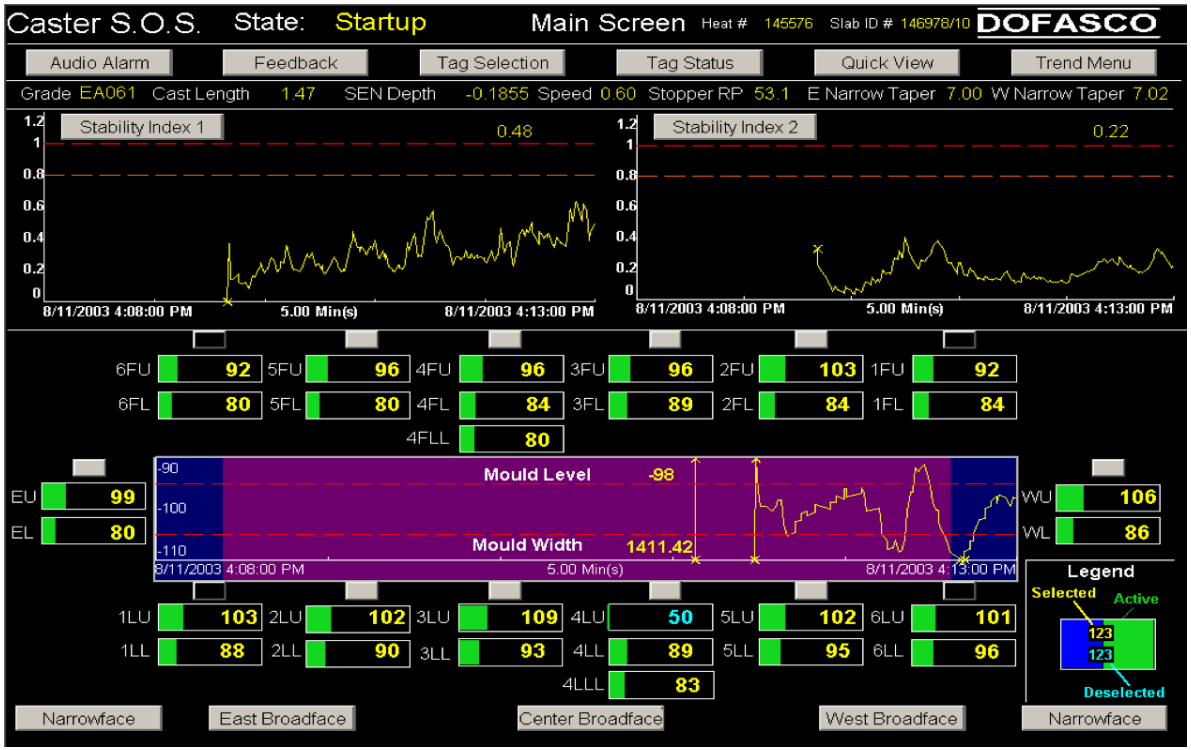


Dofasco case study: breakout

Dofasco case study: monitoring for breakouts



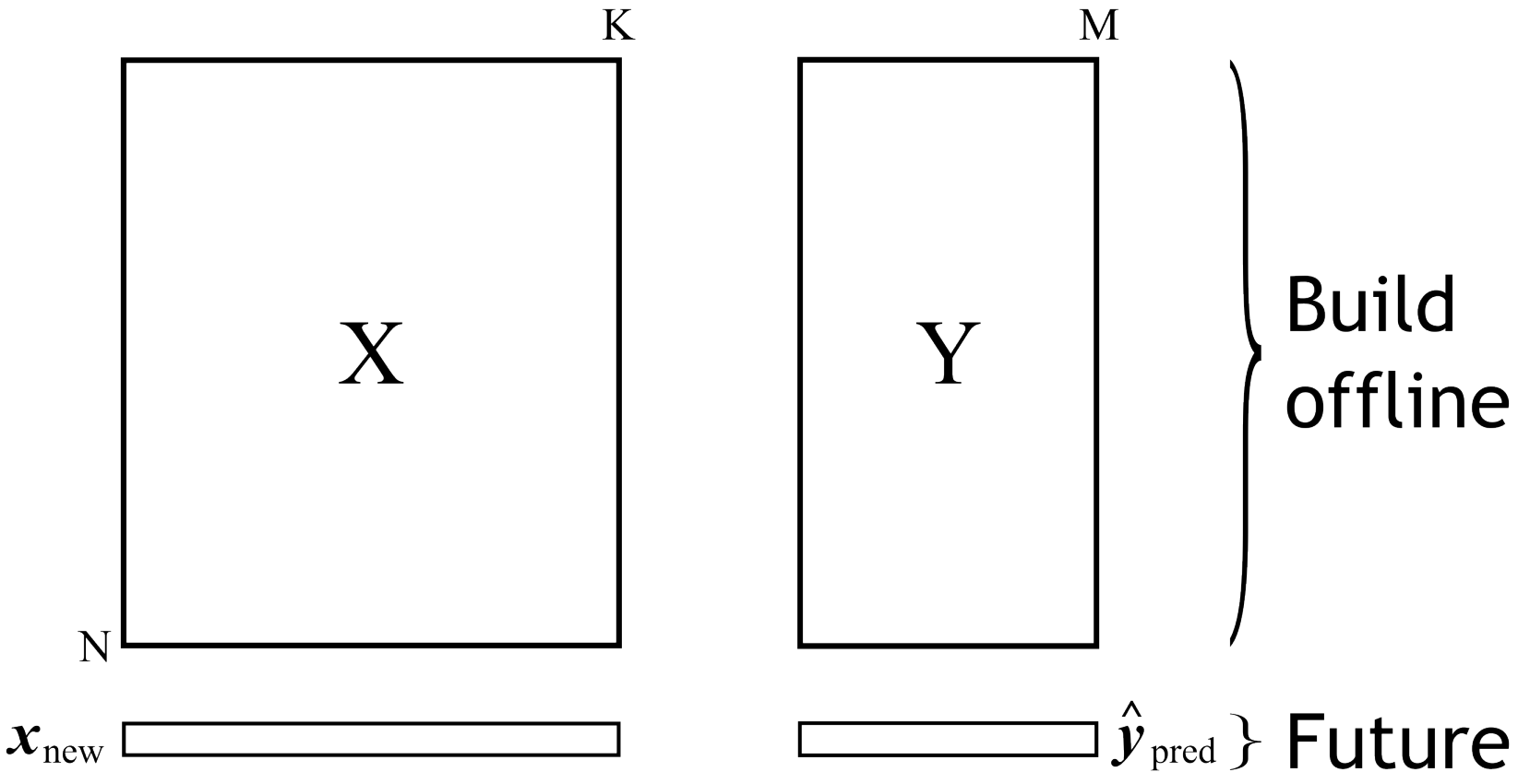
Dofasco case study: monitoring for breakouts



- Stability Index 1 and 2:
  - Hotelling's T2
  - SPE
- When alarm: shows contribution plots
- Shows real-time raw data, as operator requires it

Predictive modelling (inferential sensors)

- MLR has some serious disadvantages
  - Cannot handle missing data
  - Cannot handle strong correlations
  - MLR requires $N > K$
  - Only one y-variable at a time
  - Assumes no noise in $\mathbf{X}$, which is never true



Predictive modelling (inferential sensors)

- Inferential sensor = soft sensor
- Image data used as **X**
- Snackfood example: http://dx.doi.org/10.1021/ie020941f
- Work by Honglu Yu
  - http://digitalcommons.mcmaster.ca/opendissertations/866/

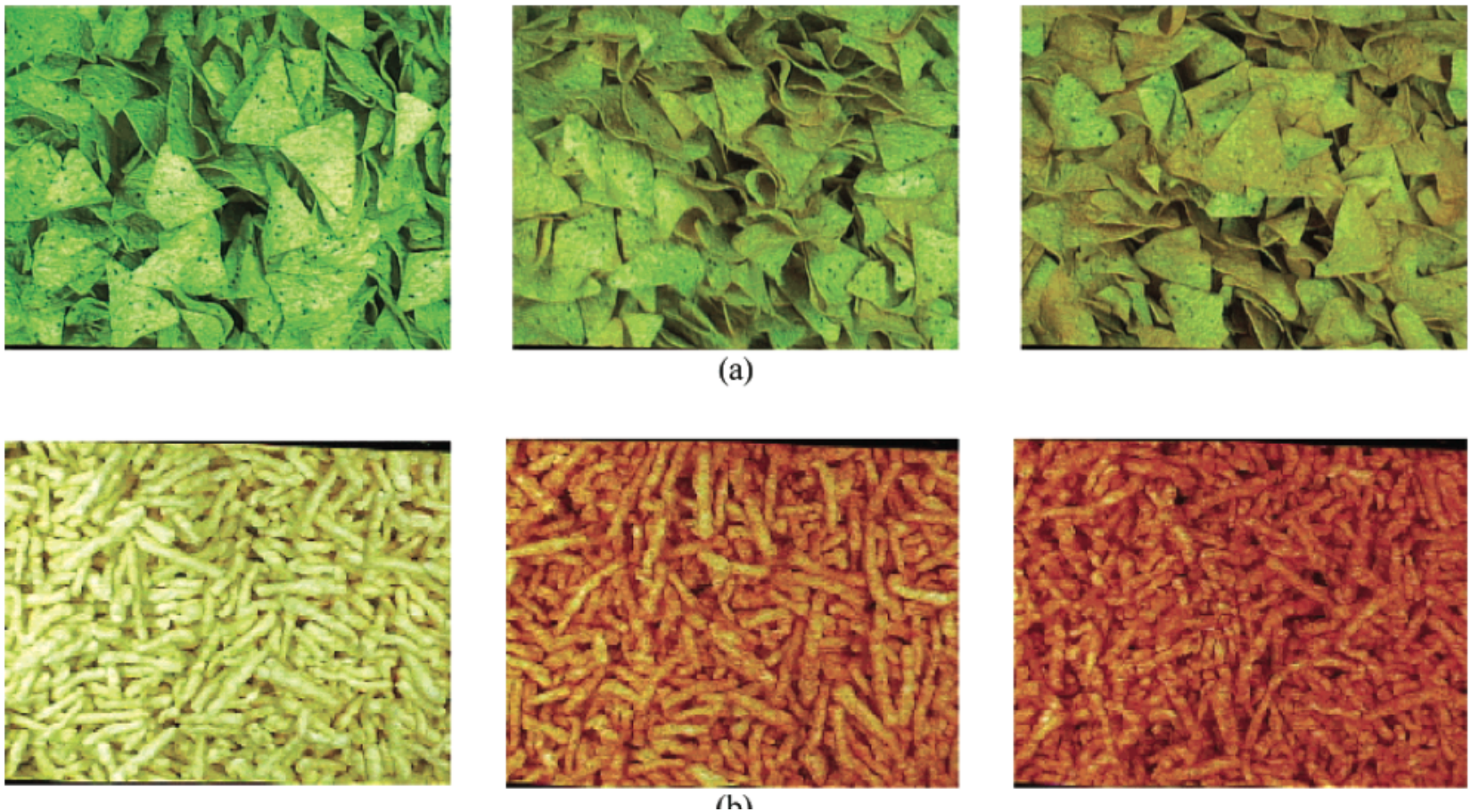


Figure 2 from the paper

Predictive modelling (inferential sensors)

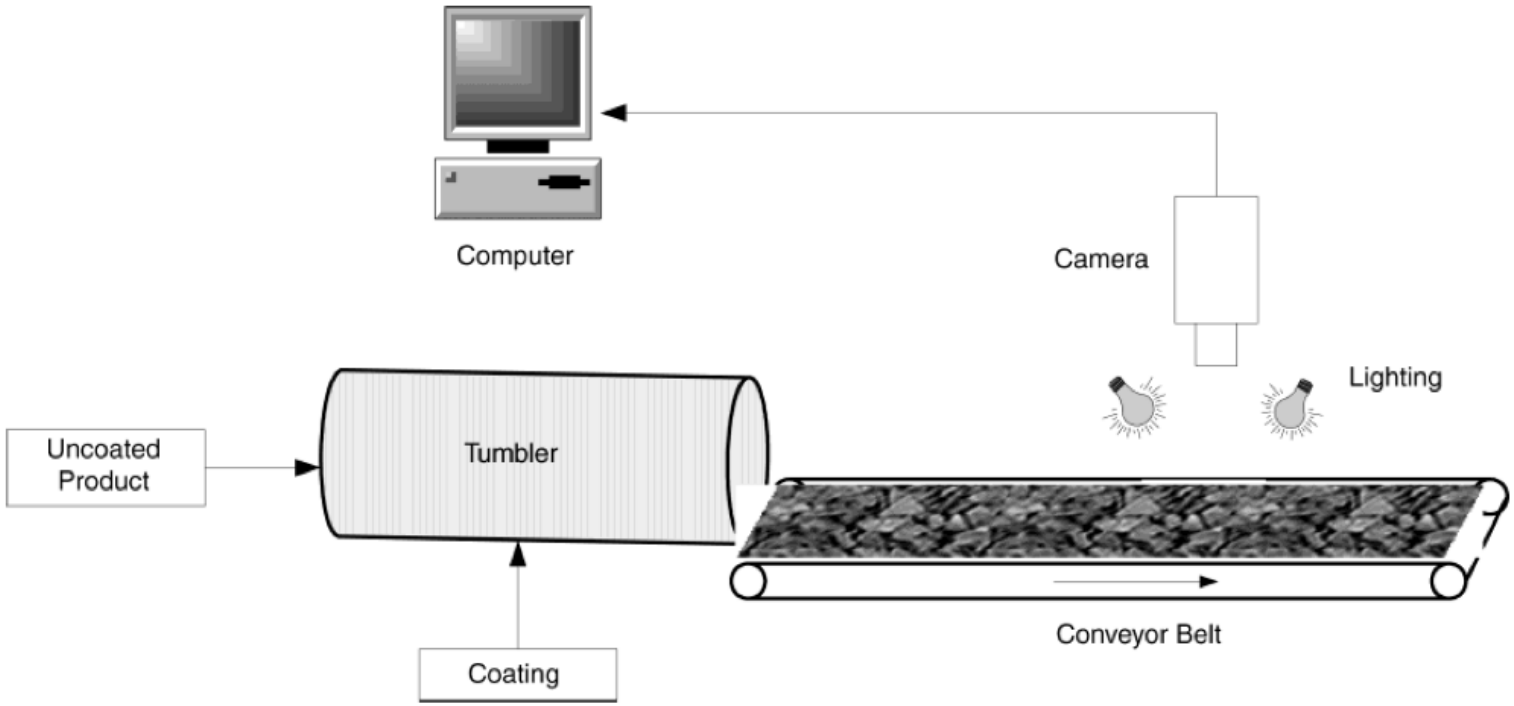


Figure 8. Schematic of the processes and imaging systems.

Figure 8 from the paper: http://dx.doi.org/10.1021/ie020941f

Predictive modelling (inferential sensors)

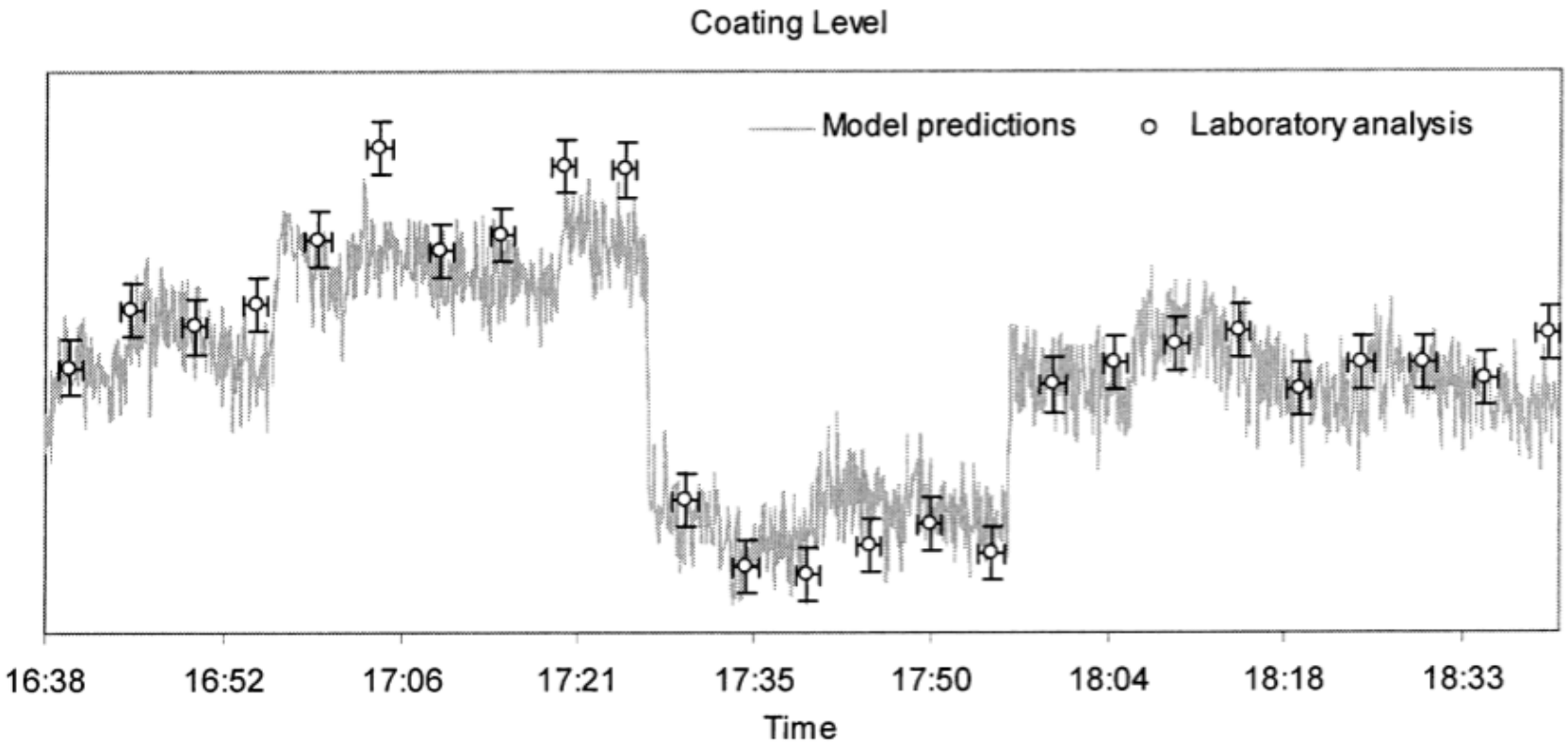


Figure 10 from the paper: http://dx.doi.org/10.1021/ie020941f

Summary: Extracting value from data

1. Improve process understanding
   - Pastry example
   - Competitor example
2. Troubleshooting process problems
   - Monomer example
   - Poor *vs* Adequate yield
3. Improving, optimizing and controlling processes
   - Pastry example
4. Predictive modelling (inferential sensors)
   - Snackfood example
5. Process monitoring
   - Dofasco example
   - Batch example