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Bayesian Approach to assign Consensus Values in PT Comparisons

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LNE
Le progrès, une passion à partager

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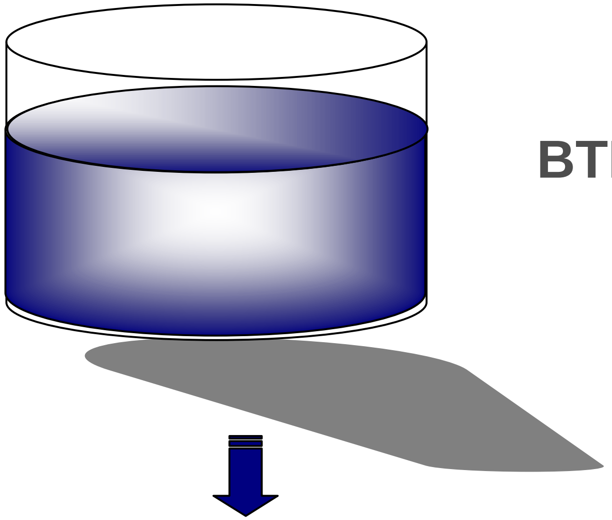
Outline

- **Framework of Proficiency Testing**
  - ✓ PT data
  - ✓ Standardized approach to assign consensus values: NF ISO 13 528
- **The proposed approach: modelling bias**
  - ✓ Methodology
  - ✓ When to introduce latent predictors of bias?
  - ✓ Statistical model
- **Estimating the model**
  - ✓ Bayesian computation of posterior distributions
  - ✓ Getting the consensus value, its associated uncertainty and bias
- **Conclusion**
- **Perspectives**

Framework of the project

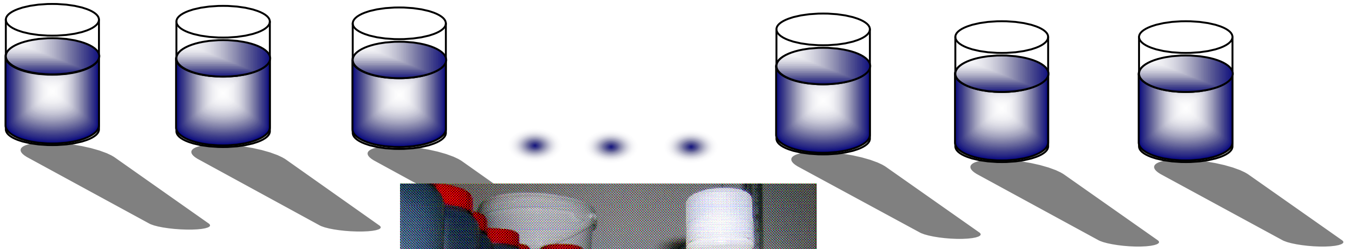
- Era-net+ European project entitled « Traceable measurements for biospecies and ion activity in clinical chemistry » (JRP 10, TRACEBIOACTIVITY)
- WP 5: PTB, SP, LNE
- Delivery 2: Evaluating a consensus value in proficiency tests.
- Funded by the European Community's Seventh Framework Programme, ERA-NET Plus, under Grant Agreement No. 217257.

Samples provided by BIPEA



BTEX, PCB, Triazines

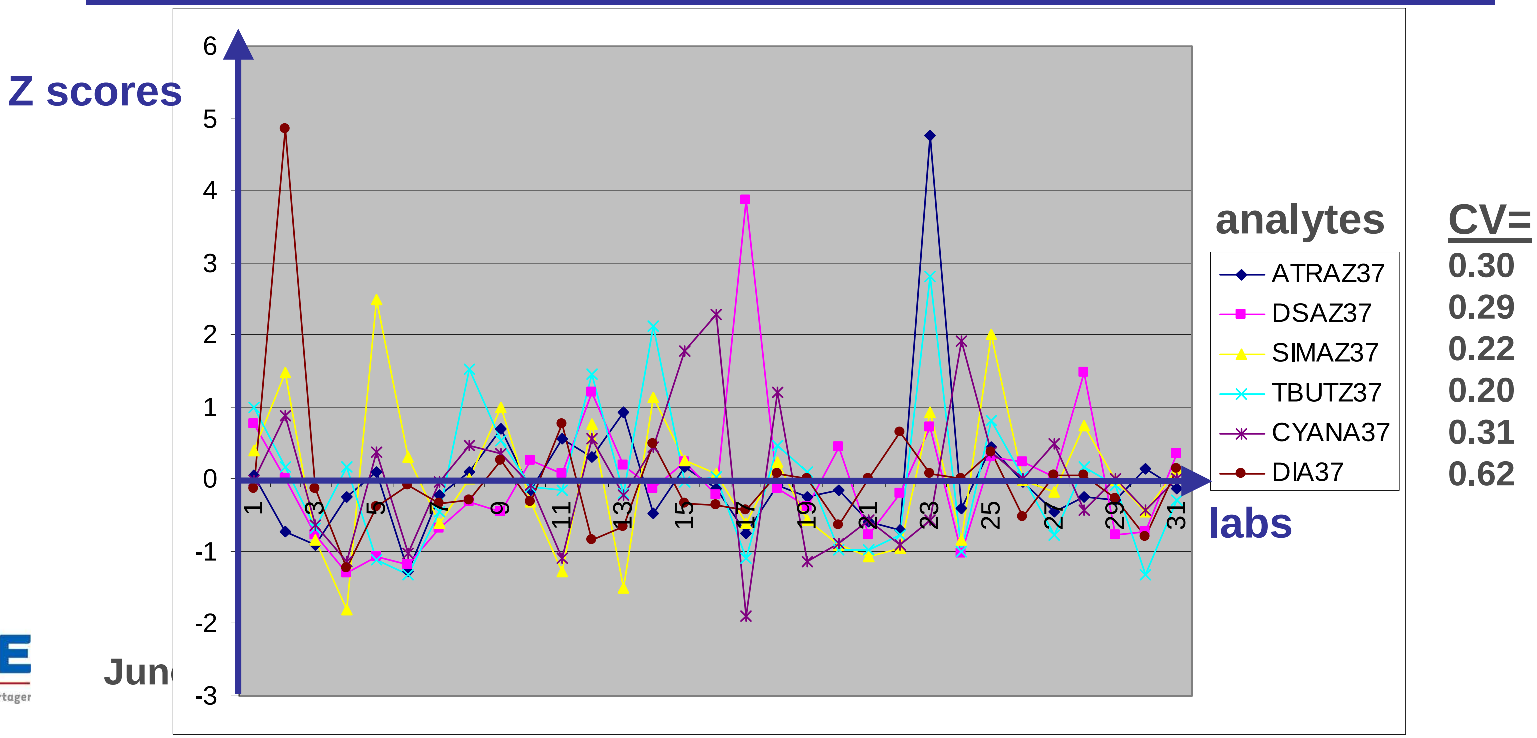
N stable and homogene samples



PT data

- PT provider: BIPEA (2nd provider in Europe)
- Measurands: concentrations of BTEX, Triazine and PCB in water
- No associated uncertainties
- 31 participating laboratories

Example: results for 6 analytes from triazine family



NF ISO 13 528

Statistical methods for use in proficiency testing by interlaboratory comparisons

5.6 Consensus value from participants [see ISO/IEC Guide 43-1:1997, A.1.1 item e)]

5.6.1 General

«With this approach, the assigned value X for the test material used in a round of a proficiency testing scheme is the <u>robust average</u> of the results reported by <u>all the participants</u> in the round, calculated using <u>Algorithm A</u> in Annex C.

<u>Other calculation methods</u> may be used in place of Algorithm A, provided that they have a sound statistical basis and the report describes the method that is used. »

NF ISO 13 528: Algorithm A

Algorithm A to compute robust means and standard deviations

Initialisation

$$x^* = x_i\text{'s median}$$

$$s^* = 1,483 \times \text{median of the } \left| x_i - x^* \right|$$

Iterate till convergence

$$x_i^* = \begin{cases} x_i^* - \delta & \text{if } x_i < x^* - \delta \\ x_i^* + \delta & \text{if } x_i > x^* + \delta \\ x_i & \text{otherwise} \end{cases}$$

$$\delta = 1,5 s^*$$

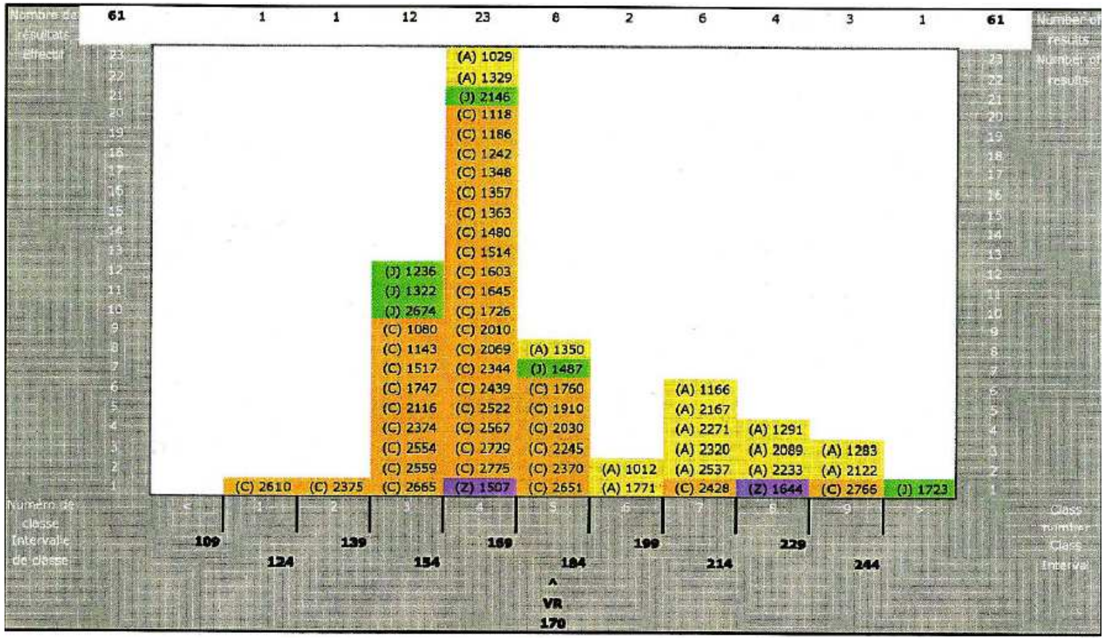
Outputs:

Consensus value: x^*

Bias: $x_i - x^*$

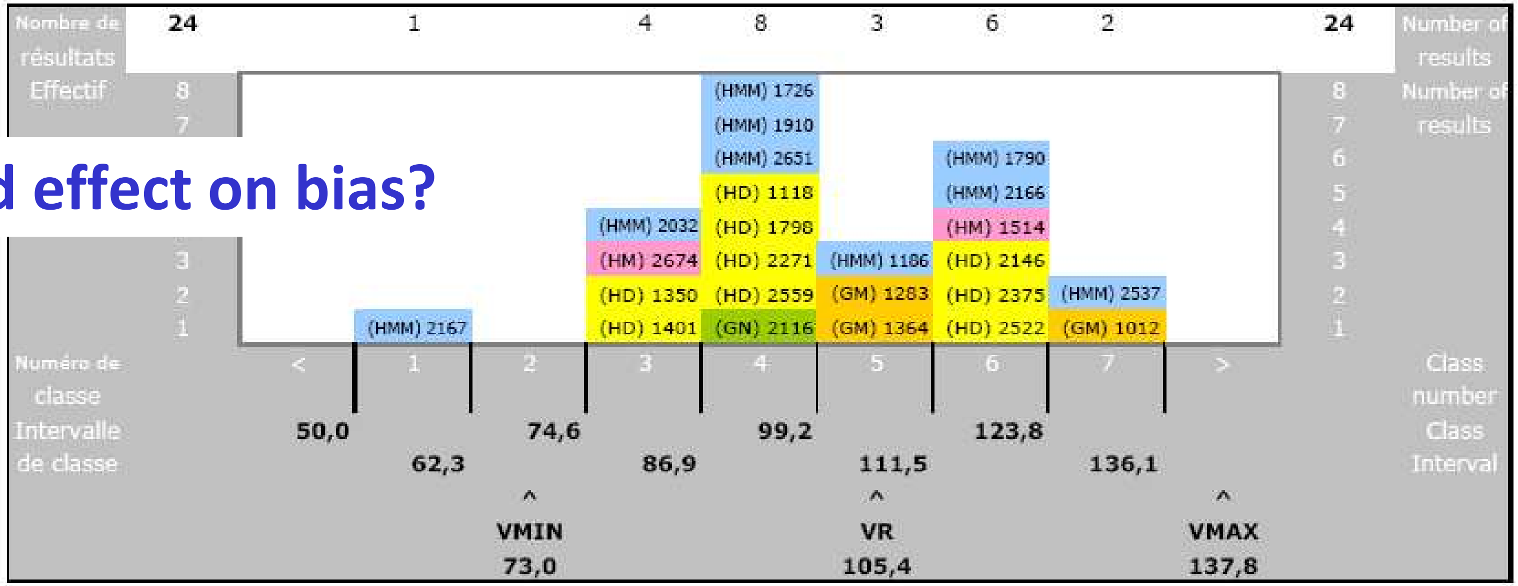
Associated uncertainty: $u_x = 1,25 \times \frac{s^*}{\sqrt{p}}$

Examples



Effect of method on bias?

Crossed effect on bias?



Overview

Proficiency testing

Measurement data
(quality assessment)

Auxiliary information
(survey)

statistical model

Bayesian estimation

consensus value,
associated uncertainty,
bias

Proposed measurement model

Modelling Bias

Consensus value

Measurement bias of laboratory *j*

$$X_j = \mu + Z_j \beta + \tau_j$$

Results

Predictors

Nature of Z_j ?

Construction of predictors

- Depends on the measurand
- Based on experts knowledge (survey,…)
- If a few number of variables can explain bias:

  → Z_j are kept as observed variables

- If several variables can explain bias:

  → the observed variables are grouped

  → Z_j are *latent variables* summarizing the observed variables

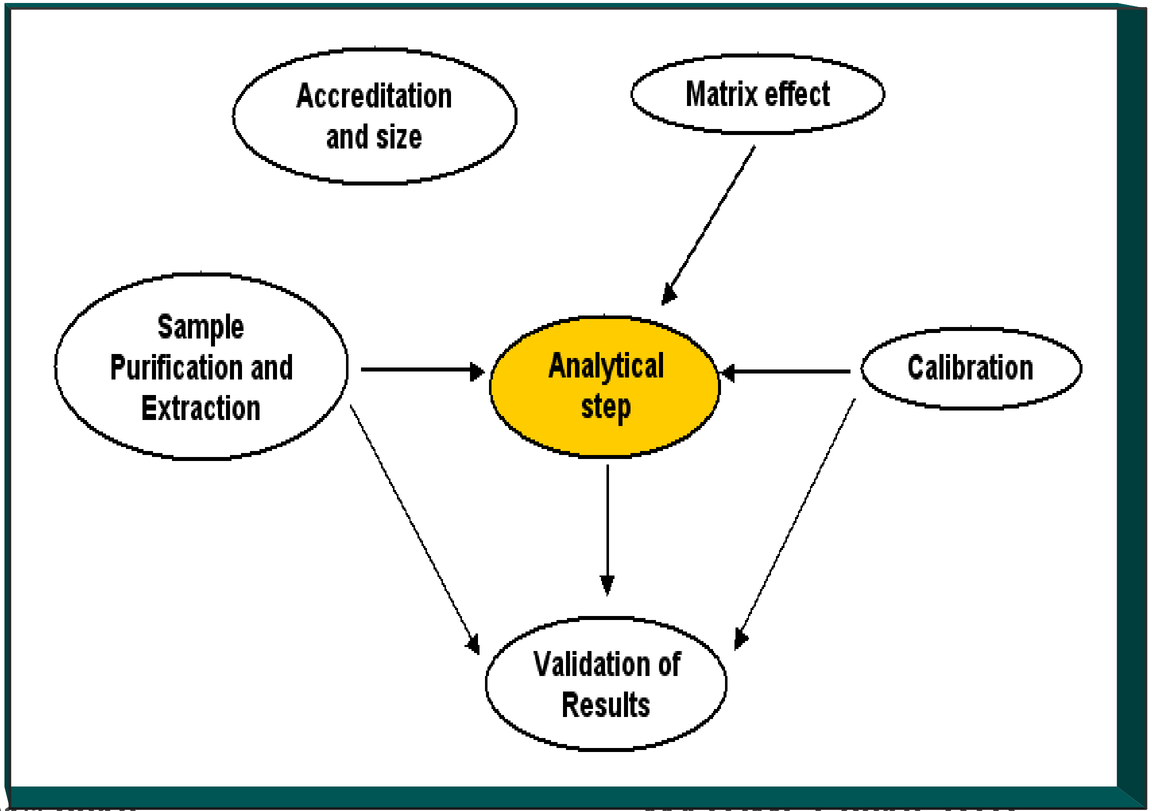
  → Z_j should capture structures in data

Steps

- Collecting measurements
- Collecting additional information on laboratories (survey)
- Converting this information into variables
  → latent variables
- Constructing a statistical model
- Estimating the model
- Validating the model

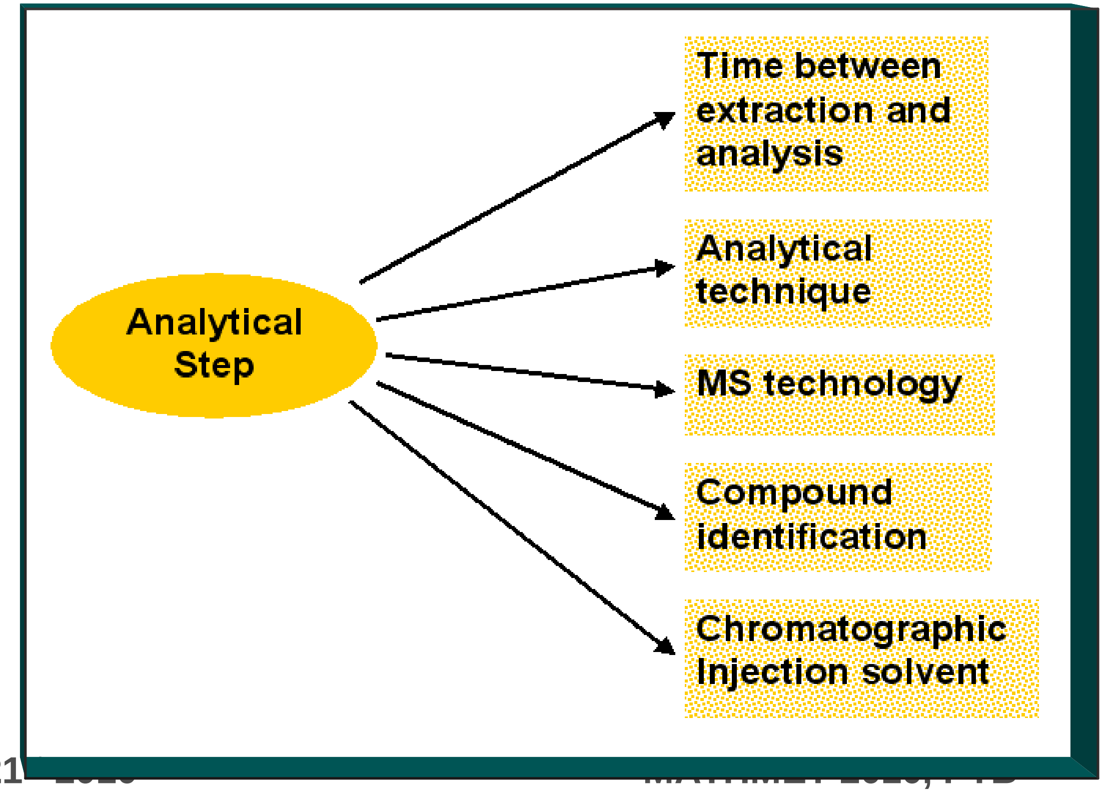
Building latent variables

- Idea: summarizing measurement process + background information on labs
- Blocks = latent (unobserved) concepts, variables

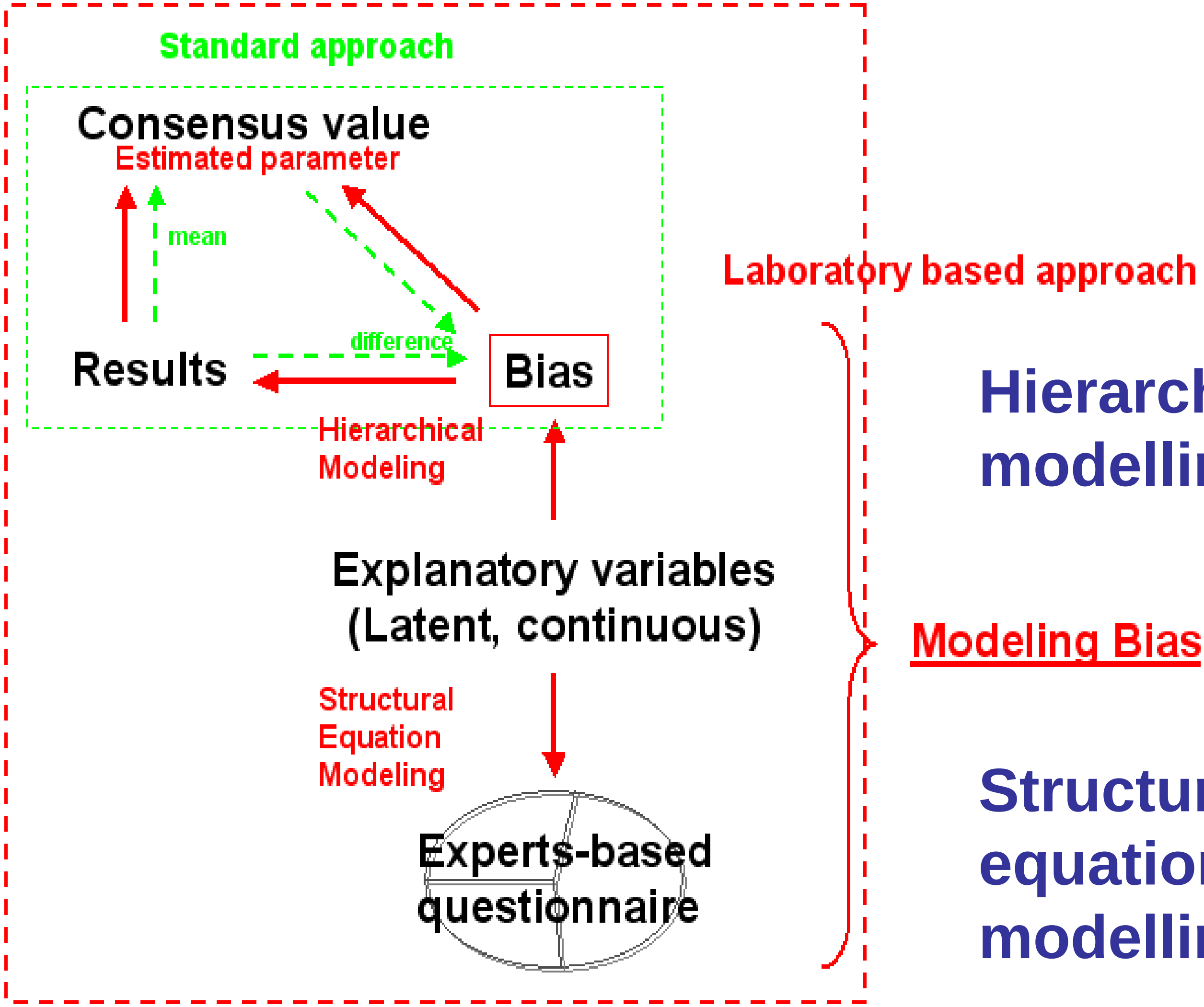


Links between questions and blocks

- Latent concepts are measured on observed variables (the questions)
- Example:



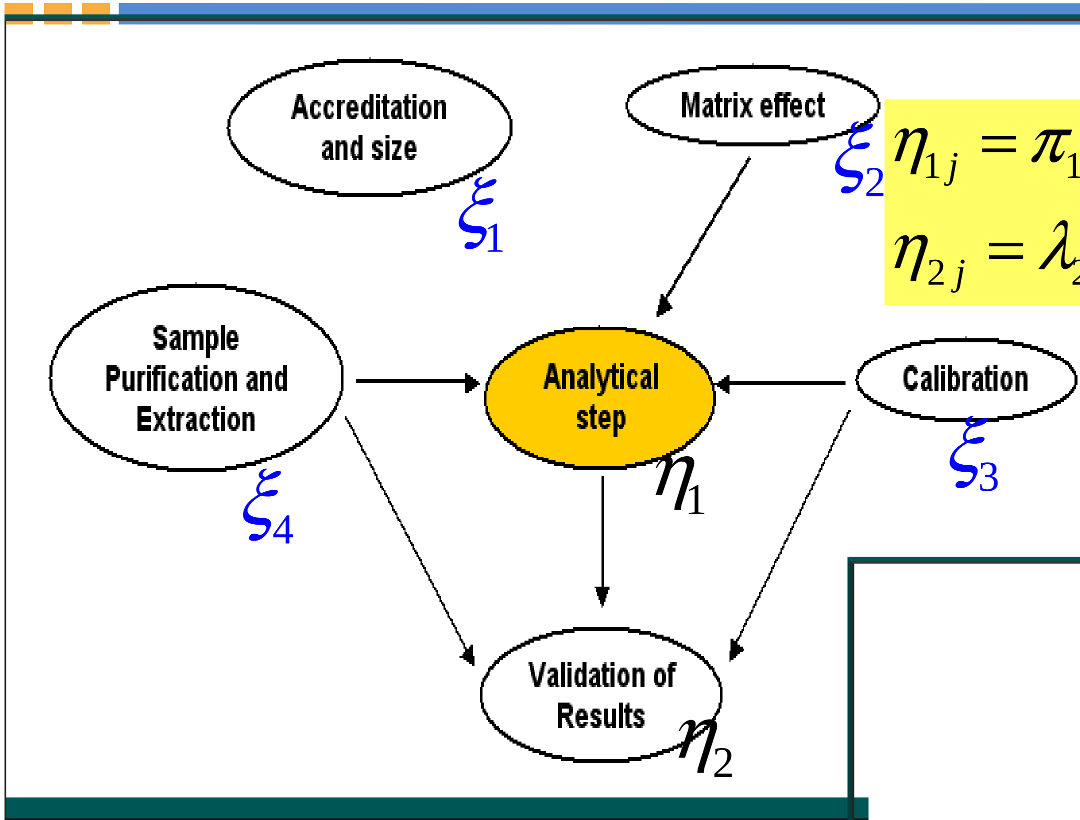
Structure of the model



Hierarchical modelling

Structural equation modelling

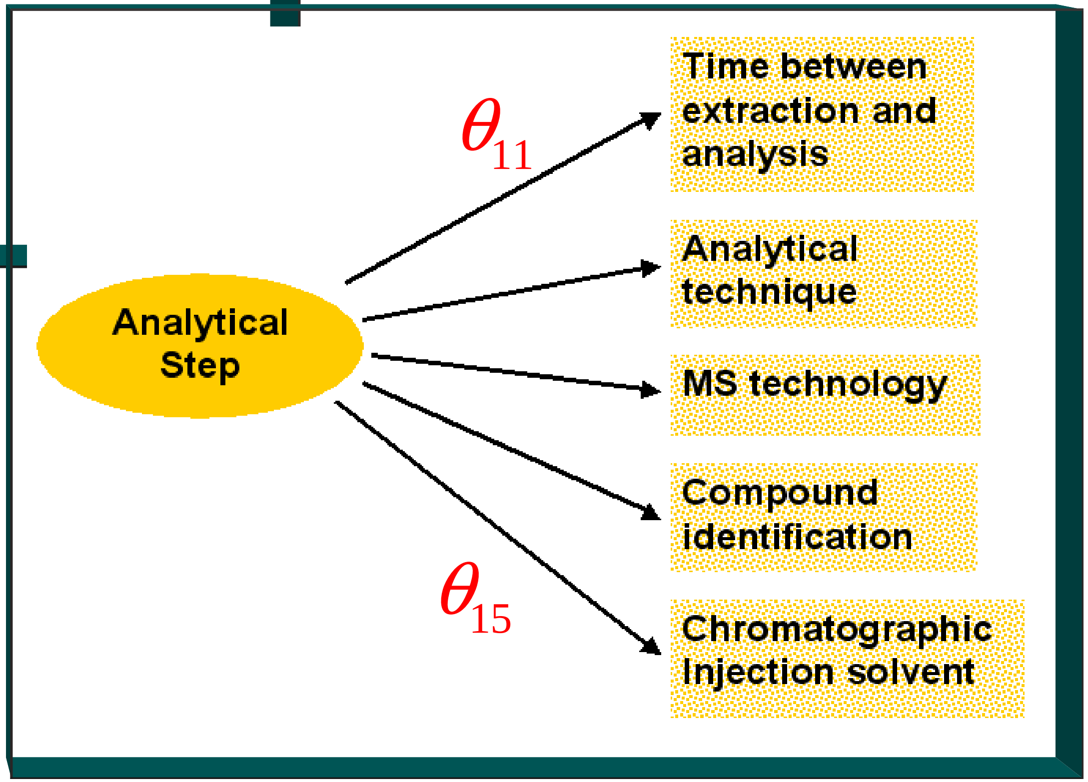
Structural equation modelling



$$\eta_{1j} = \pi_{12}\eta_{2j} + \lambda_{12}\xi_{2j} + \lambda_{13}\xi_{3j} + \lambda_{14}\xi_{4j} + \delta_{1j}$$

$$\eta_{2j} = \lambda_{23}\xi_{3j} + \lambda_{24}\xi_{4j} + \delta_{2j}$$

(Simultaneous equations)



$$y_{1j} = \theta_{11}\eta_{1j} + \varepsilon_{1j}$$

$$\ldots$$

$$y_{5j} = \theta_{15}\eta_{1j} + \varepsilon_{5j}$$

Complete model

Consensus value

Results

Bias

$$X_j = \mu + Z_j\beta + \nu_j$$

Auxiliary data

$$Y_j = Z_j\theta + \varepsilon_j$$

$$H_j = Z_j\Lambda + \delta_j$$

SEM

Endogeneous latent variables

Model inference: Bayesian approach

- To take into account prior information on parameters (correlations, variances)
- Estimation algorithm based on posterior conditional distributions (MCMC)
- Iterating:
  - ✓ Imputation of latent variables
  - ✓ Posterior sampling of parameters

Proposed Gibbs algorithm to estimate SEM

Initialisation : $\theta^0, \Sigma_\varepsilon^0, \Lambda^0, \Sigma_\delta^0, \Phi^0$

A l'itération t :

1. imputation des variables latentes :
   $Z^t \sim Z|Y, \theta^{t-1}, \Sigma_\varepsilon^{t-1}, \Lambda^{t-1}, \Sigma_\delta^{t-1}, \Phi^{t-1}$
2. **réduction des variables latentes** : soit Z^{*t} la VL réduite
3. $\Sigma_\varepsilon^t \sim \Sigma_\varepsilon|Y, Z^{*t}, \theta^{t-1}, \Lambda^{t-1}, \Sigma_\delta^{t-1}, \Phi^{t-1}$
4. $\theta^t \sim \theta|Y, Z^{*t}, \Sigma_\varepsilon^t, \Lambda^{t-1}, \Sigma_\delta^{t-1}, \Phi^{t-1}$
5. $\Sigma_\delta^t \sim \Sigma_\delta|Y, Z^{*t}, \Lambda^{t-1}, \theta^t, \Sigma_\varepsilon^t, \Phi^{t-1}$
6. $\Lambda^t \sim \Lambda|Y, Z^{*t}, \Sigma_\delta^t, \theta^t, \Sigma_\varepsilon^t, \Phi^{t-1}$
7. $\Phi^t \sim \Phi|Y, Z^{*t}, \theta^t, \Sigma_\varepsilon^t, \Lambda^t, \Sigma_\delta^t$

Imputation of latent variables

Let $\Theta = \{\theta, \Sigma_\varepsilon, \Lambda, \Sigma_\delta, \Phi\}$

$$[Z|Y,\Theta] \propto \prod_{i=1}^{n} [Z_i|Y_i,\Theta] \propto \prod_{i=1}^{n} [Y_i|Z_i,\Theta]\,[Z_i|\Theta]$$

- $[Y_i|Z_i,\Theta] = [Y_i|Z_i,\theta,\Sigma_\varepsilon]$
- $[Z_i|\Theta] = [Z_i|\Lambda,\Sigma_\delta,\Phi] \sim \mathcal{N}\left(0,\Sigma_Z\right)$

Results:

$$Z_i|Y_i,\theta,\Sigma_\varepsilon,\Lambda,\Sigma_\delta,\Phi \sim \mathcal{N}\left(D\theta\Sigma_\varepsilon^{-1}Y_i, D\right)$$

$D = \theta\Sigma_\varepsilon^{-1}\theta^t + \Sigma_Z^{-1}.$

Posterior conditional distributions

Let $\Theta = \{\theta, \Sigma_\varepsilon, \Lambda, \Sigma_\delta, \Phi\}$

$$
\begin{aligned}
[\Theta | Y, Z] &\propto [Y, Z | \Theta] [\Theta] \\
&\propto [Y | Z, \Theta] [Z | \Theta] [\Theta]
\end{aligned}
$$

- $[Y | Z, \Theta] = [Y | Z, \theta, \Sigma_\varepsilon]$
- $[Z | \Theta] = [Z | \Lambda, \Sigma_\delta, \Phi] = [H | \Xi, \Lambda, \Sigma_\delta] [\Xi | \Phi]$
- $[\Theta] = [\theta, \Sigma_\varepsilon] [\Lambda, \Sigma_\delta] [\Phi]$

$$
[\Theta | Y, Z] \propto \underbrace{[Y | Z, \theta, \Sigma_\varepsilon] [\theta, \Sigma_\varepsilon]}_{[\theta, \Sigma_\varepsilon | Y, Z]} \; \underbrace{[H | \Xi, \Lambda, \Sigma_\delta] [\Lambda, \Sigma_\delta]}_{[\Lambda, \Sigma_\delta | Y, Z]} \; \underbrace{[\Xi | \Phi] [\Phi]}_{[\Phi | Z]}
$$

Posterior conditional distributions

Conjugate models
Normal/Gamma

$$Y_k = \theta_k Z + \varepsilon_k, \quad Y_k \sim N\left(\theta_k Z, \Sigma_\varepsilon\right)$$

$$\theta_k | Y, Z, \Sigma_\varepsilon \sim \mathcal{N}\left(D_k A_k, \Sigma_{\varepsilon k} D_k\right)$$

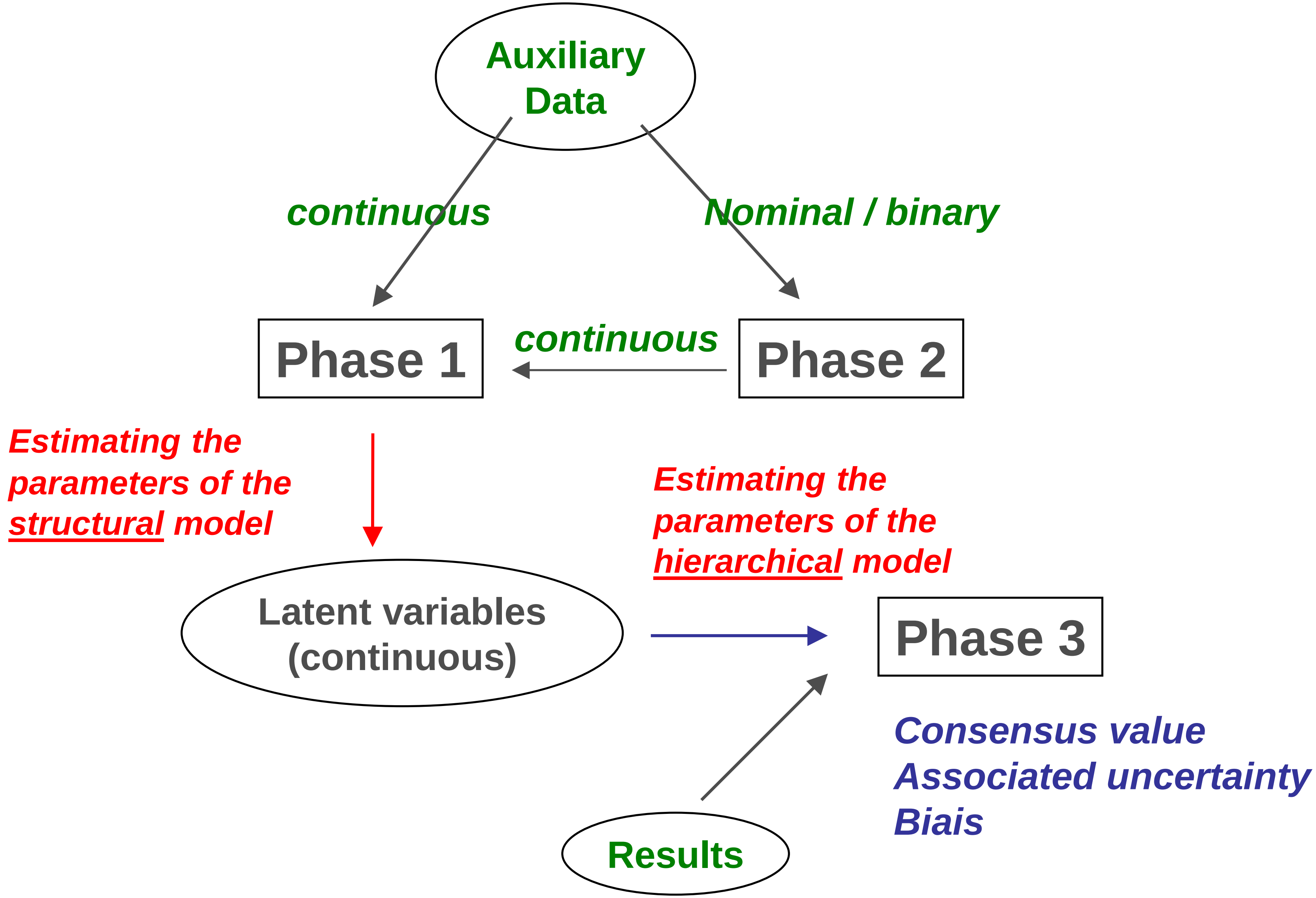
$$D_k = \left(Z^t Z + \Sigma_{0\varepsilon}^{-1}\right)^{-1}$$
$$A_k = Z^t Y_k + \Sigma_{0\varepsilon}^{-1} \theta_{0k}$$

$$H_k = \Lambda_k Z_k + \delta_k, \quad H_k \sim N\left(\Lambda_k Z_k, \Sigma_{\delta k}\right)$$

$$\Lambda_k | Z, \Sigma_{\delta k} \sim \mathcal{N}\left(D_k A_k, \Sigma_{\delta k} D_k\right)$$

$$D_k = \left(Z^t Z + \Sigma_{0\delta}^{-1}\right)^{-1}$$
$$A_k = Z^t H_k + \Sigma_{0\delta}^{-1} \Lambda_{0k}$$

Estimation of the model: 3 phases



Conclusion

- New approach to compute consensus values and their associated uncertainties
  - ✓ Modelling bias
  - ✓ Modelling structures in auxiliary data

- To propose different models from ANOVA to SEM to handle structures in the auxiliary information.

- Collaborative work between experts and statisticians.

- Model inference in progress for nominal auxiliary data.

Perspectives

- To test the approach with SEM on water pollutants when the statistical tool works with nominal data
- To adapt the model for creatinine data (another structure of the auxiliary information)