The case of metrology: estimation of calibration functions with a small number of data

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MESURES ET RÉFÉRENCES

VECTEUR DE COMPÉTITIVITÉ
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Le progrès, une passion à partager

Context and goal of the project

- Working group involving industrials, metrologists and statisticians
- Aims at providing guidelines to metrologists and industrials for an efficient implementation of Bayesian calibration in the field of measurement
- Project supported by the French national metrology research program

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The Bayesian choice

- The measurement result is the probability distribution associated with the measurand according to the VIM
- Metrologists often have a strong expertise, knowledge and historical data on their measurement models

- Bayesian inference provides posterior distributions for quantities of interest
- Bayesian framework allows to incorporate all the prior knowledge to the measurement into the statistical model

[O'Hagan 2014]

Example of balance calibration

Five mass standards are used to calibrate the balance

Balance calibration : Data

Point	Balance response Y_i^{obs}		Standard X_i (mg)	
	indication (y_i^{obs})	Standard uncertainty	value (x_i)	
i=1	1.9000000e-02	38.47	50.019	
i=2	1.8000800e+02	57.71	100.008	
i=3	8.2001900e+02	96.43	1 000.019	
i=4	4.6400480e+03	195.32	5 000.048	
i=5	1.9280056e+04	407.34	20 000.056	

Bayesian “classical” regression

Normal linear regression model:

$$Y^{obs} = X\beta + \varepsilon, \quad \varepsilon \sim N(0, \boldsymbol{\Sigma_Y})$$

X_i : true value of standard *i*

Y_i^{obs} : indication given by the device

- Prior distribution $\boldsymbol{P}(\boldsymbol{\beta}, \boldsymbol{\Sigma_Y})$ determined accordingly to the knowledge available on these parameters. Normal Inver Gamma distribution is commonly used

- Likelihood : $Y_i^{obs} \mid \beta, x_i \sim N\left(\beta_0 + \beta_1 x_i, \tau_{\varepsilon_{y_i}}^{-1}\right)$

$$P\left(Y^{obs} = y^{obs} \mid B = \beta, X = x\right) = \prod_{i=1}^{5} \frac{1}{\sqrt{\tau_{\varepsilon_{y_i}}^{-1}}\sqrt{2\pi}} \exp\left(-\frac{\left(y_i^{obs} - \left(\beta_0 + \beta_1 x_i\right)\right)^2}{2\tau_{\varepsilon_{y_i}}^{-1}}\right)$$

- Posterior distribution

$$P(\beta, \boldsymbol{\Sigma_Y} | \boldsymbol{y^{obs}}) \propto \boldsymbol{P}(\boldsymbol{\beta}, \boldsymbol{\Sigma_Y}) \times \boldsymbol{l}(\boldsymbol{y^{obs}} | \boldsymbol{\beta}, \boldsymbol{\Sigma_Y})$$

[Klauenberg 2014]

Let’s come back to the definition of calibration

2.39 (6.11) *VIM*

calibration

*operation that, under specified conditions, in a first step, establishes a relation between the quantity values **with measurement uncertainties** provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication*

Balance calibration : full data

Point	Balance response Y_i^{obs}		Standard X_i(mg)	
	indication (y_i^{obs})	Standard uncertainty	value (x_i)	Standard uncertainty
i=1	1.9000000e-02	38.47	50.019	21.1
i=2	1.8000800e+02	57.71	100.008	27.76
i=3	8.2001900e+02	96.43	1 000.019	50.59
i=4	4.6400480e+03	195.32	5 000.048	84.13
i=5	1.9280056e+04	407.34	20 000.056	140.49

The uncertainty associated with the value x_i is often available and non negligible !

Errors in variables models

- The alternative is then to use models that consider both uncertainties associated with the two variables
- Errors in variables models:

Functional relationships between the true quantities: $Y = X\beta$, β unknown

Error models relating observations and true values: $x_i^{obs} = X_i + \varepsilon_i \quad y_i^{obs} = Y_i + \varepsilon_i'$

with $\varepsilon_i \sim \boldsymbol{N}(\boldsymbol{0}, \boldsymbol{\Sigma_X})$ and $\varepsilon_i' \sim N(0, \boldsymbol{\Sigma_Y})$

[Fuller 1987]

- Standard ISO/TS 28037:2010 *Determination and use of straight-line calibration functions* is providing algorithms for straight line calibration in presence of complex structure of uncertainty, but not in a Bayesian Framework
- Bayesian analysis of such regression models have been studied only for straight line case or for applications in other fields than metrology

[Reilly 1981]

Notations

$K \geq 1$: number of standards

X_k : true value of standard k

$J_k \geq 1$: number of replicates of indications regarding standard k

$J = \sum_{k=1}^{K} J_k$: total number of indications

$Y_{k,j}^{obs}$: replicate j of the indication given by the instrument regarding standard k

$f(.,\boldsymbol{\beta}) : \mathbb{R} \to \mathbb{R}$: functional relationships where $\boldsymbol{\beta}$ is a vector of real numbers,

$$\underbrace{\mathbf{1}_n}_{(n,1)} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}, \quad \underbrace{\boldsymbol{X}}_{(J,1)} = \begin{pmatrix} X_1 \mathbf{1}_{J_1} \\ \vdots \\ X_K \mathbf{1}_{J_K} \end{pmatrix}, \quad \underbrace{\boldsymbol{Y}_k^{obs}}_{(J_k,1)} = \begin{pmatrix} Y_{k,1} \\ \vdots \\ Y_{k,J_k} \end{pmatrix}, \quad \underbrace{\boldsymbol{Y}^{obs}}_{(J,1)} = \begin{pmatrix} \boldsymbol{Y}_1^{obs} \\ \hline \vdots \\ \hline \boldsymbol{Y}_k^{obs} \\ \hline \vdots \\ \hline \boldsymbol{Y}_K^{obs} \end{pmatrix}.$$

$$and \quad \underbrace{\boldsymbol{Y}}_{(J,1)} = \boldsymbol{f}(\boldsymbol{X},\boldsymbol{\beta}) = \begin{pmatrix} f(X_1,\boldsymbol{\beta})\mathbf{1}_{J_1} \\ \vdots \\ f(X_K,\boldsymbol{\beta})\mathbf{1}_{J_K} \end{pmatrix}$$

In case of a straight line calibration function: $\underbrace{\boldsymbol{\beta}}_{(2,1)} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \quad f(X_k,\boldsymbol{\beta}) = \beta_0 + \beta_1 X_k$

Bayesian calibration model

Prior distributions :

$\boldsymbol{X} \sim \boldsymbol{\pi}(\varphi_{\boldsymbol{X}})$ knowledge about X often provided by certificate through
$\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{X}^{ref}, \boldsymbol{\Sigma}_{\boldsymbol{X}})$

$\boldsymbol{\beta} \sim \boldsymbol{\pi}(\varphi_{\boldsymbol{\beta}})$ e.g. for a straight line : $\boldsymbol{\beta} = \begin{pmatrix}\beta_0 \\ \beta_1\end{pmatrix} \sim \mathcal{N}(\begin{pmatrix}\mathbf{0} \\ \mathbf{1}\end{pmatrix}, \boldsymbol{\Sigma}_{\boldsymbol{\beta}})$

Under the normality assumption :

$$\boldsymbol{Y}^{obs}/\boldsymbol{X} = \boldsymbol{x} \sim \mathcal{N}(\boldsymbol{f}(\boldsymbol{X}, \boldsymbol{\beta}), \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{Y}^{obs}}}_{(J,J)}),$$

$\boldsymbol{\Sigma}_{\boldsymbol{Y}^{obs}} \sim \boldsymbol{\pi}(\varphi_{\boldsymbol{\Sigma}_{\boldsymbol{Y}^{obs}}})$, $\boldsymbol{\Sigma}_{\boldsymbol{Y}^{obs}}$ may be known through uncertainty budget

Bayesian inference

Let's assume that $\boldsymbol{\Sigma}_{\boldsymbol{\beta}}$ and $\boldsymbol{\Sigma}_{\boldsymbol{Y}^{obs}}$ are known, *which is a very common situation*

Posterior distribution :

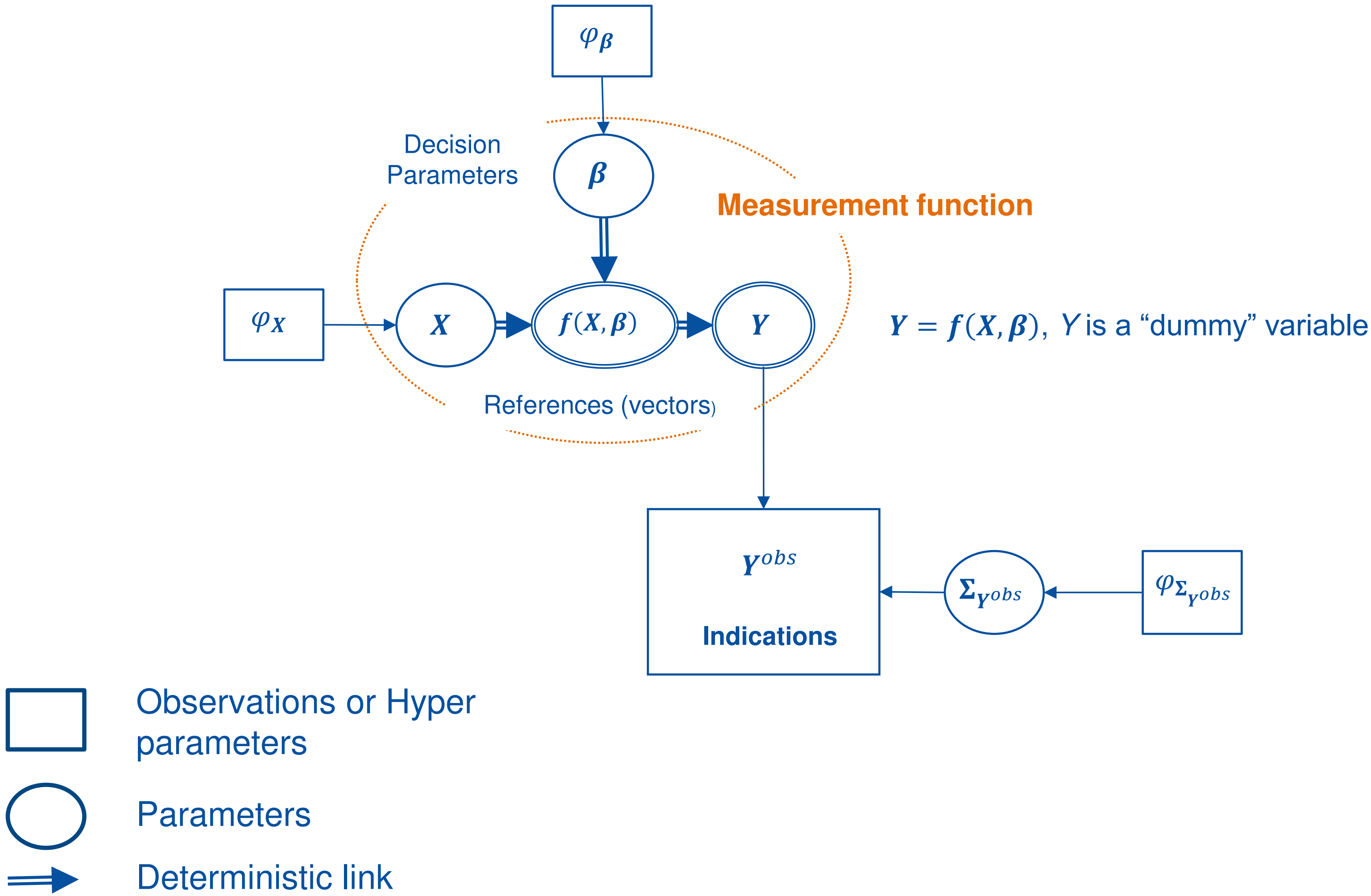
$$P(\beta, X|Y^{obs}) \propto l\left(Y^{obs}\middle|\beta, X\right)P(\beta)P(X)$$

Marginalised posterior distribution :

$$P\left(\beta|Y^{obs}\right) = \int_X P\left(\beta, X|Y^{obs}\right)d(X)$$

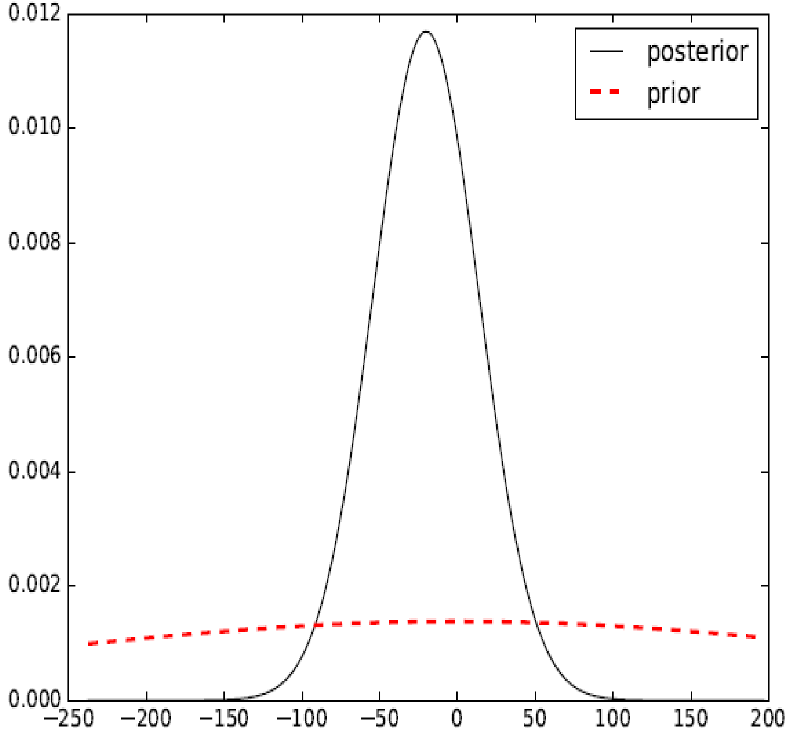
In practice, apart from the Normal assumption for straight line calibration models, the posterior distribution of the parameters β is not explicit and should be simulated through a MCMC algorithm.

Representation of the balance calibration model : DAG

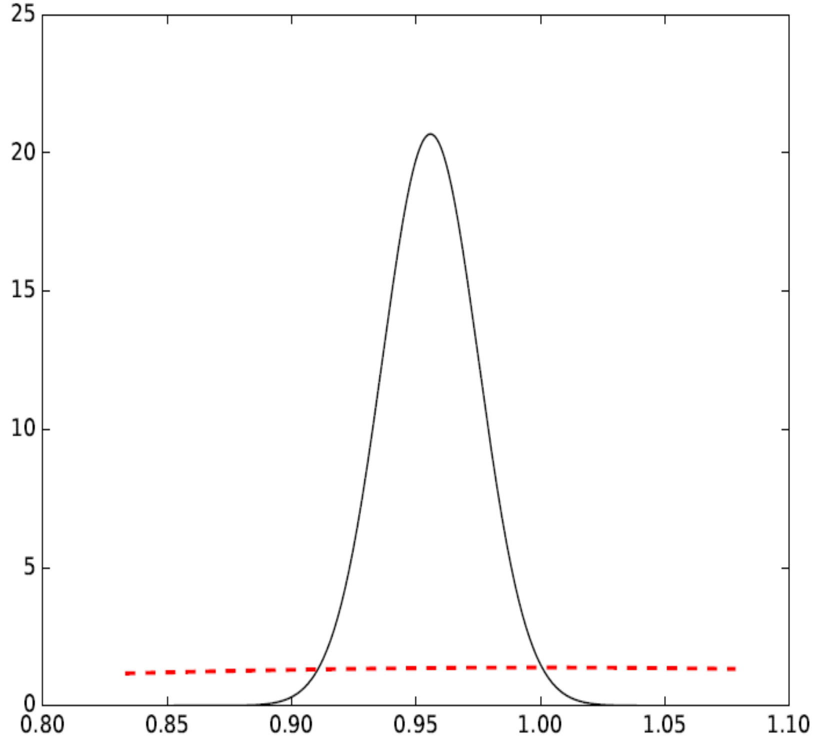


Results for the parameters β

Prior $\beta_0 \sim N(0, 288^2)$ $\beta_1 \sim N(1, 0.288^2)$



β_0

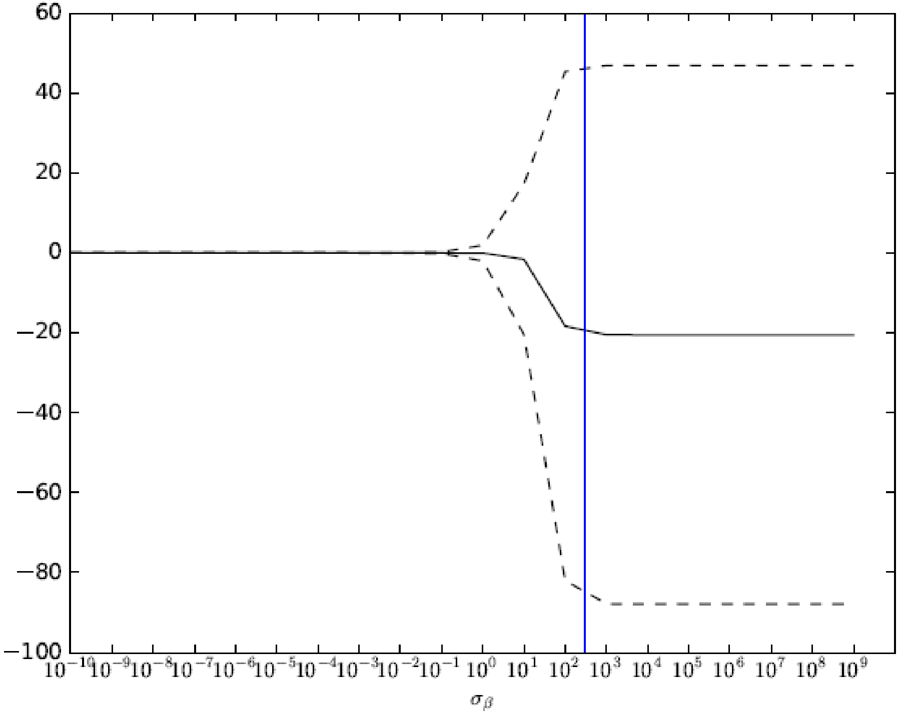


β_1

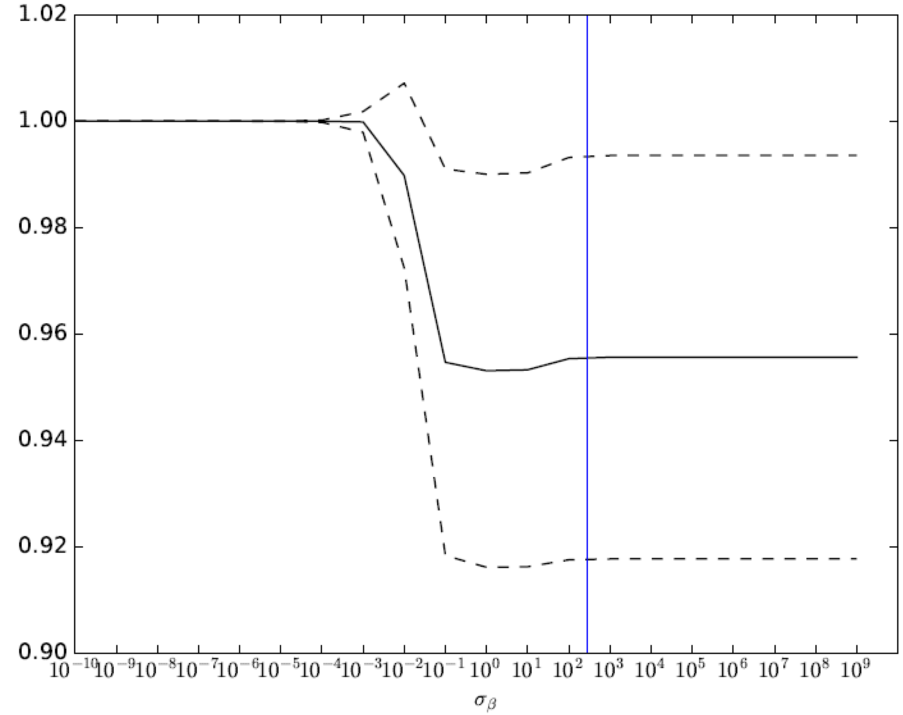
Posterior	mean	std	2.5 perc	97.5 perc
β_0	-20	34	-87	47
β_1	0.96	0.019	0.92	0.99

95% credible intervals of the posterior distribution of β_0 and β_1 in function of the standard deviation of the prior distribution

β_0

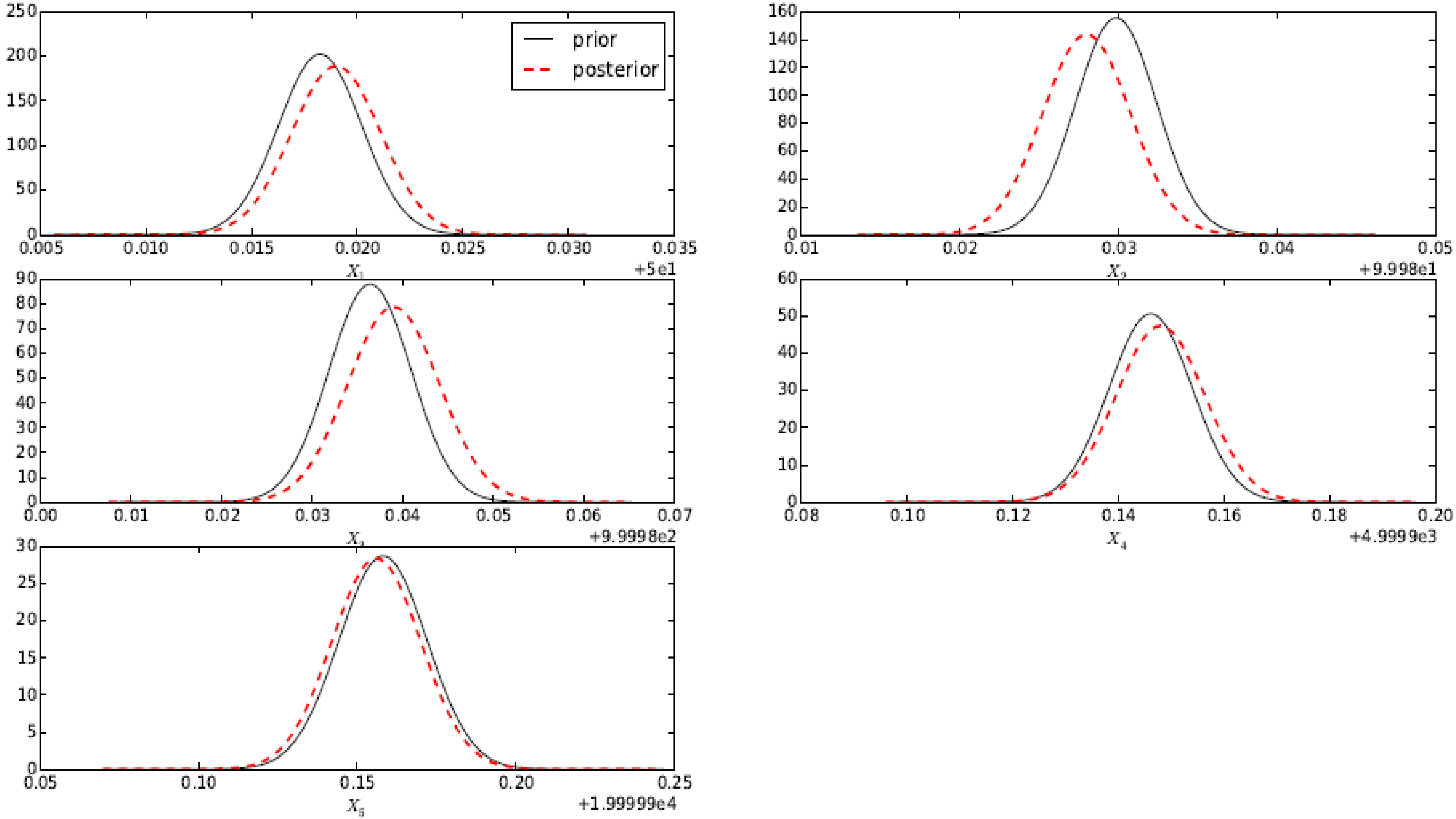


β_1



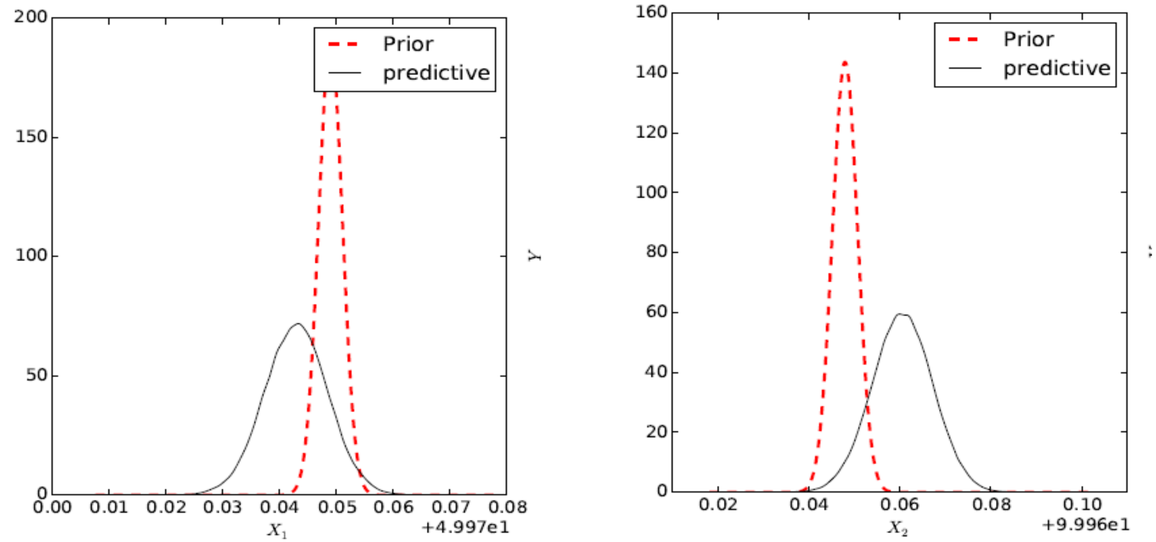
Blue line is the current choice of variance parameter

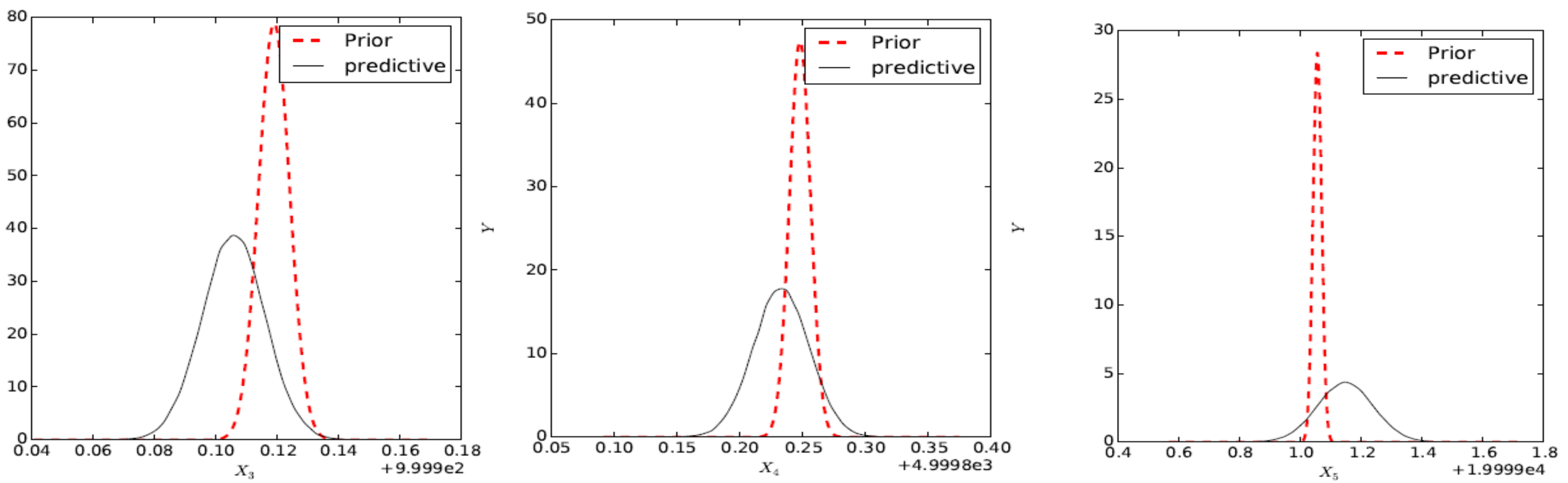
Prior and posterior probability distributions of X



Model checking by cross validation

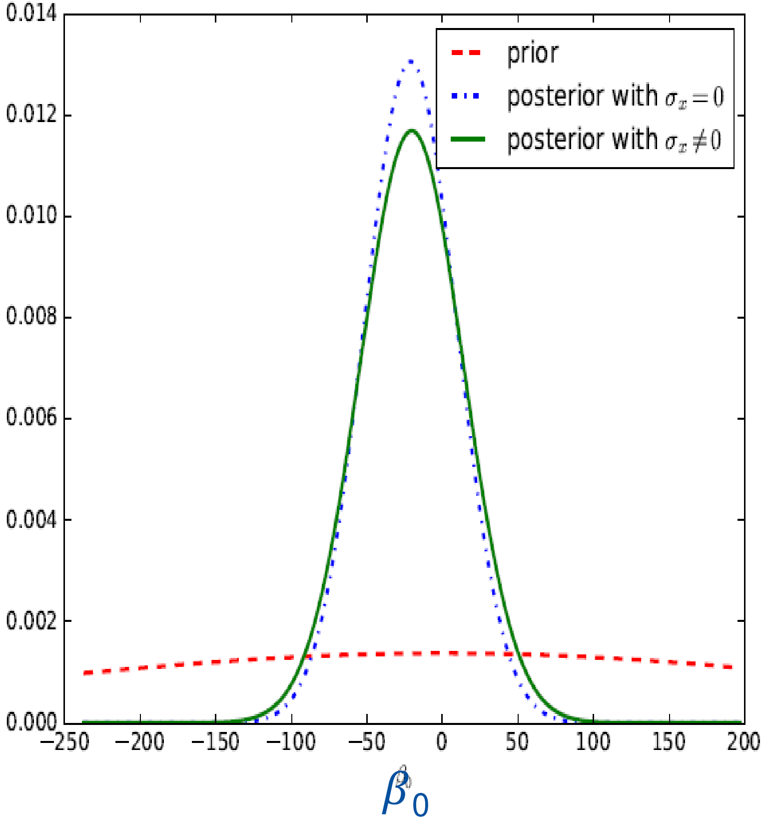
Leave one out for each X_k and estimate of its predictive posterior distribution comparing with its prior one

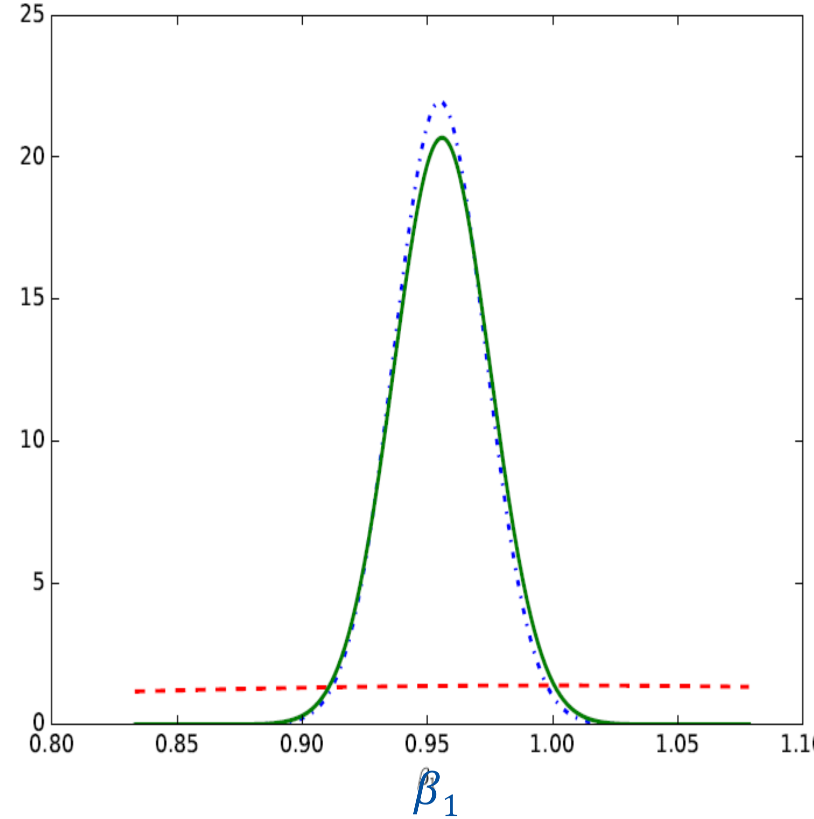




Comparison of posterior distribution

Posterior distribution of β obtained by Bayesian classical regression (green curve) and new Bayesian calibration model (dashed blue curve) under same prior





Posterior	mean	std	2.5 p	97.5 p
β_0	-20	34	-87	47
$\beta_0 \sum_X = 0$	-21	31	-81	39

Posterior	mean	std	2.5 p	97.5 p
β_1	0,96	0,019	0,92	0,99
$\beta_1 \sum_X = 0$	0.95	0.018	0.92	0.99

Second step of the calibration : prediction

Given Y_0^{obs} a new indication written on the balance, let's predict X^{new} the value of the quantity that is measured :

$$P\left(\beta, X, X^{new} | Y_0^{obs}, Y^{obs}\right) \propto l\left(Y_0^{obs}, Y^{obs} \middle| \beta, X, X^{new}\right) P(\beta, X) P(X^{new})$$
$$\propto l\left(Y_0^{obs} \middle| \beta, X^{new}\right) P\left(\beta | Y^{obs}\right) P(X^{new})$$

$\Sigma_{Y_0^{obs}}$ is assumed to be known

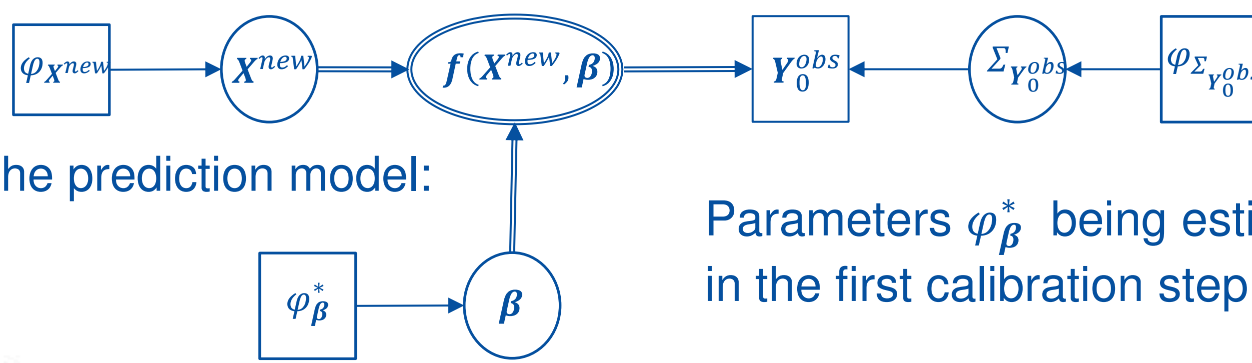
Marginal posterior distribution for X^{new} is then obtained by :

$$P\left(X^{new} | Y_0^{obs}, Y^{obs}\right) = \int l\left(Y_0^{obs} \middle| \beta, X^{new}\right) P\left(\beta | Y^{obs}\right) P(X^{new}) d\beta$$

In practice due to industrial and philosophical constraints X^{new}'s conditional posterior given X and β is considered :

$$E\left[\pi\left(X^{new} \middle| Y_0^{obs}, X, \beta\right) \middle| Y^{obs}\right] = \int \pi\left(X^{new} \middle| Y_0^{obs}, X, \beta\right) \pi\left(\beta, X \middle| Y_0^{obs}, Y^{obs}\right) d\beta dX$$

DAG of the prediction model:

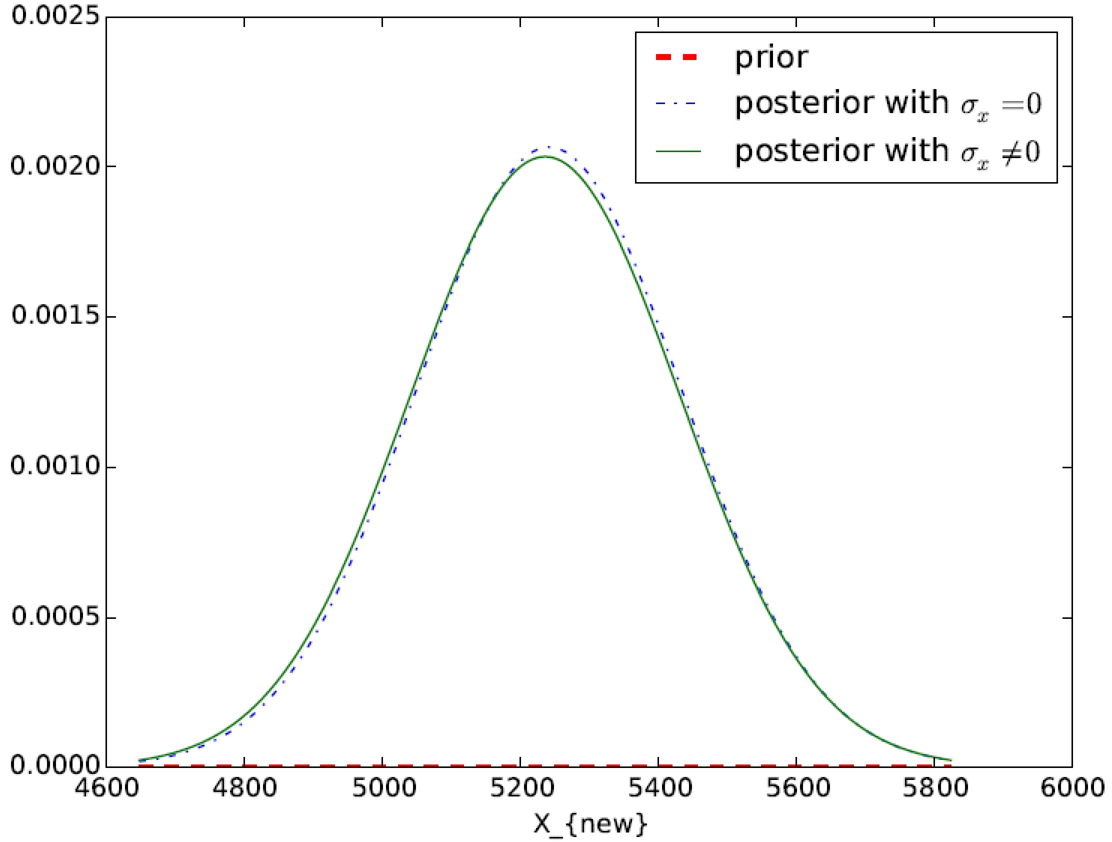


Parameters φ_β^* being estimated in the first calibration step

Comparison of predictions

Numerical example : Y_0^{obs} = 4984, $\sigma_{Y_0^{obs}}$ = 159 , and Prior $X^{new} \sim N(0, large)$

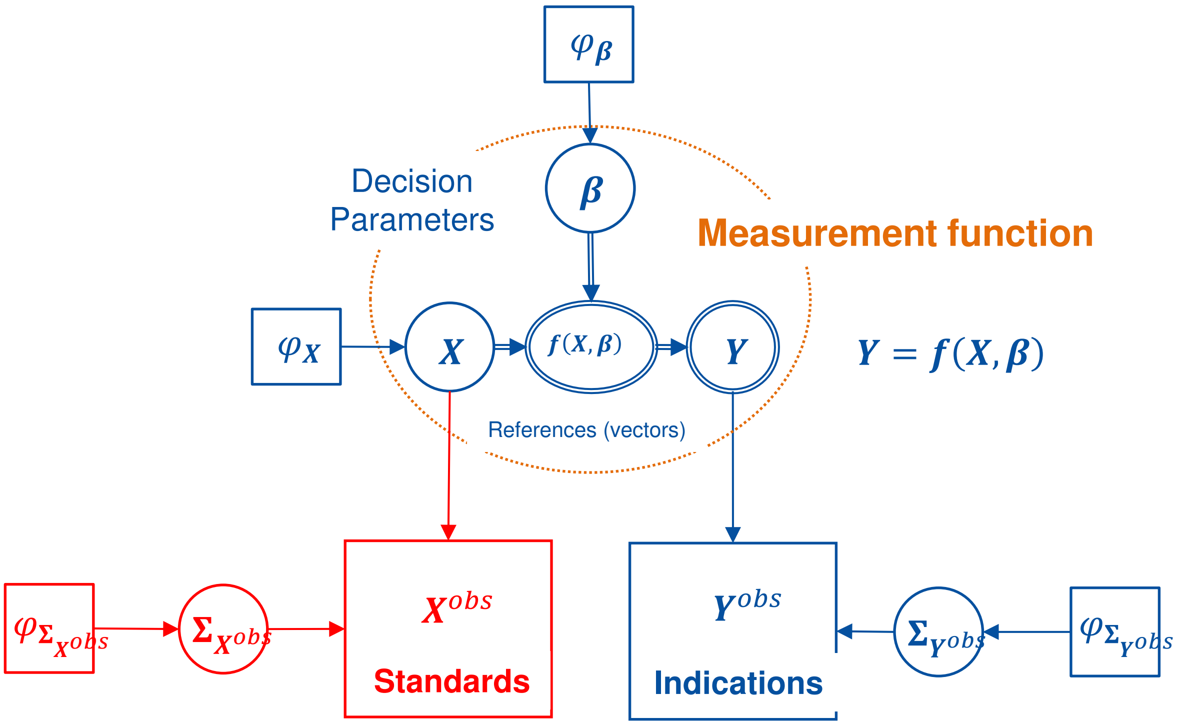
Posterior distribution of X^{new} obtained by Bayesian classical regression (green curve) and new Bayesian calibration model (dashed blue curve) under same prior



Extension of the Bayesian calibration model

In other situations, the standard is also observed during the first calibration step. This leads to a second observation equation :

$X^{obs}/X = x \sim \mathcal{N}(X, \underbrace{\Sigma_{X^{obs}}}_{(I,I)})$, with $\Sigma_{X^{obs}} \sim \pi(\varphi_{\Sigma_{X^{obs}}})$



Conclusion : advantages of this calibration model

- Bayesian calibration approach has the advantage to take into account prior knowledge, in particular past calibration data of the same device
- Model that allows to take into account **both uncertainties associated with the standard and the indication** for more reliable estimation of the calibration parameters
- Flexible model **suited for different calibration situations**
- The straight line case can be generalized to deal with polynomial calibration functions
- Analytic solution for the posterior estimates is available in case of straight line calibration (via Laplace approximation) otherwise implementation of MCMC algorithm on winbugs/R/Python

References

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Thank you for your attention