Accounting for the variability of experimental data when calibrating mechanical constitutive models

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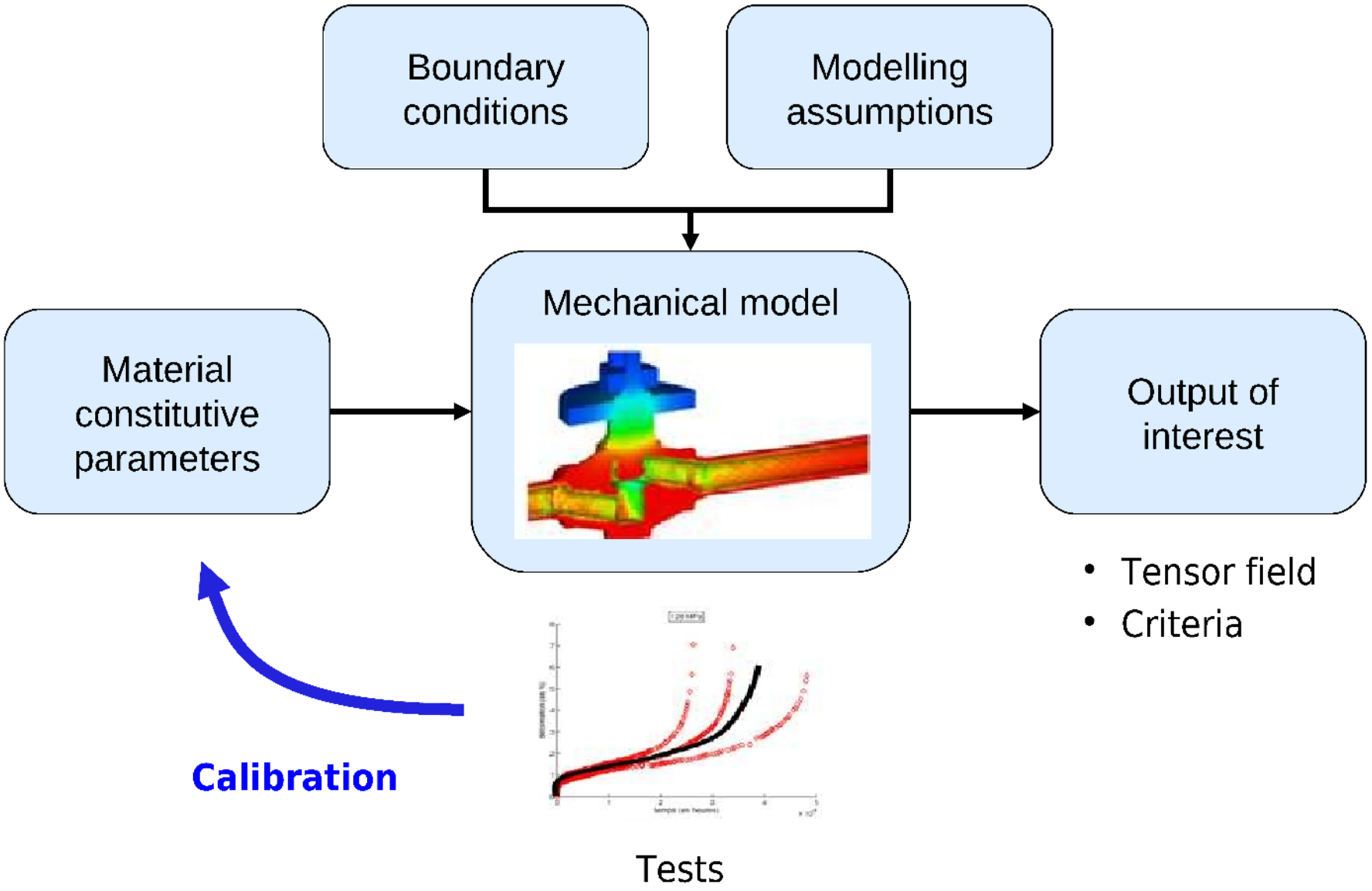
CHANGER L'ÉNERGIE ENSEMBLE

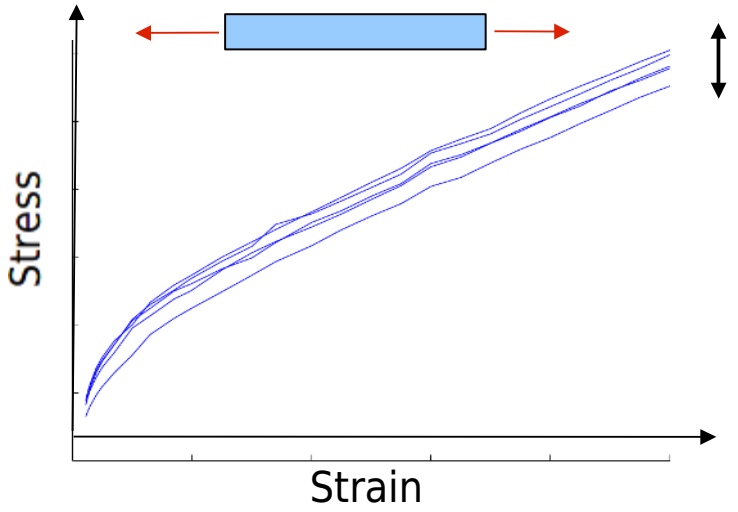
Numerical simulation of a component



Identification of a constitutive model (2)

Usually the calibration process aims at determining the « best » set of constitutive parameters (best estimate). It is often obtained by (nonlinear) least squares.

Then the best estimate feeds the component numerical model in order to compute a mechanical output of interest. However the experimental data may be significantly scattered, making it possible to erroneously skip unfavourable scenarios.



Hence it is important to account for the material variability when identifying a constitutive model

Problem statement

Objective: “Account for the experimental variability when calibrating the constitutive model.”

Two possible answers:

1. Determine specific sets of parameters corresponding to envelope curves
   → Provide a domain of variation of the final mechanical response (under monotonicity assumptions)
2. Infer a probabilistic constitutive model from the data
   → Propagate uncertainty through the mechanical model

Constraints:

- Prescribed physical-based parametric models
- Few experimental data
- No prior knowledge on the parameters (only broad intervals)

Outline

1. Classical deterministic model calibration
2. Determination of envelope constitutive models
3. Probabilistic model calibration

Constitutive model and experimental curves

We consider a constitutive model under the general form:

$$y^{sim}(t, \boldsymbol{d}) \;=\; f(t, \boldsymbol{d}, \boldsymbol{\theta})$$

where:

- t is an evolution variable (e.g. the time or a relevant state variable)
- $\boldsymbol{d}$ is a vector of fixed and known environment parameters (e.g. temperature, pressure)
- $\boldsymbol{\theta} := \{\theta_1, \ldots, \theta_p\}$ is a vector of model parameters that have to be calibrated from experimental data

We assume that we have obtained *n* experimental curves:

$$\mathcal{Y}^{exp} \;:=\; \{y_1^{exp}(t, \boldsymbol{d}_1), \ldots, y_n^{exp}(t, \boldsymbol{d}_n)\}$$

Prediction error

In practice the postulated model never perfectly fits the measurements. In other words, for each experimental curve there exists an error term:

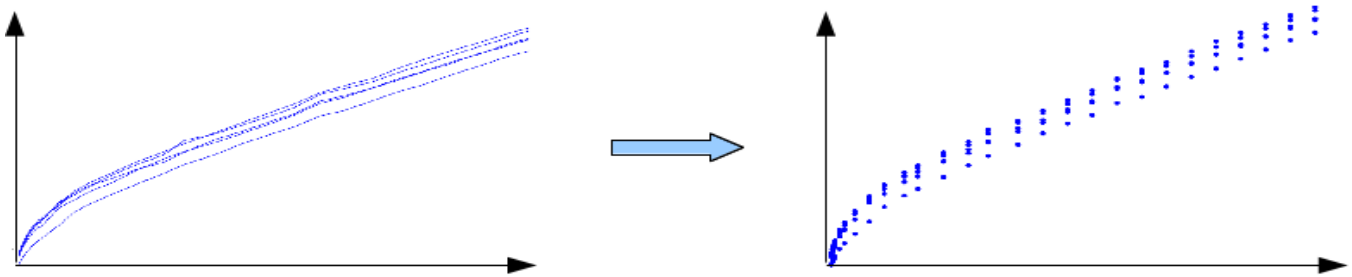
$$y_i^{exp}(t, \boldsymbol{d}_i) = f(t, \boldsymbol{d}_i, \boldsymbol{\theta}) + Err_i(t)$$

Several sources of error can be identified:

- Model inadequacy. The selected model f differs from a « true » unknown model h, which depends on $\boldsymbol{\theta}$ but also on other parameters $\boldsymbol{\lambda}$ (hidden variables).
- Material dispersion. It is an intrinsic dispersion due to variations of microstructure, composition, etc. This is taken into account by assigning a specific set $\boldsymbol{\theta}_i$ to each representative volume element.
- Measurement error.

Least squares-based calibration

It is necessary to discretize the various experimental curves in order to solve the minimization problem. We denote by $\mathcal{T}_i := \{t_{i,1}, \ldots, t_{i,m_i}\}$ the chosen subdivision of the *i*-th curve.



Least squares minimization.

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\mathbb{R}^p} \left(\sum_{i=1}^{n} \sum_{j_i \in \mathcal{T}_i} \left(f(t_{j_i}, \boldsymbol{d}_i, \boldsymbol{\theta}) - y_i^{exp}(t_{j_i}, \boldsymbol{d}_i) \right)^2 \right)$$

The problem is solved using iterative schemes, e.g. Levenberg-Marquardt.

2. Determination of envelope constitutive models

Objective

In addition to the least squares curve, determine “pessimistic” and “optimistic” curves in order to border the (scattered) data.

Precisely, find two sets of parameters which lead to simulated curves that overestimate and underestimate a given amount of experimental points, respectively.

Assuming the « monotonicity » of the mechanical model of the component, this will make it possible to estimate a domain of variation of the output of interest due to the experimental dispersion.

Quantile curves

Reminder: the error between a simulated curve and the *i*-th experimental curve is denoted by:

$$e_i(t, \boldsymbol{\theta}) \;=\; y_i^{exp}(t, \boldsymbol{d}_i) \;-\; f(t, \boldsymbol{d}_i, \boldsymbol{\theta}) \qquad , \quad i = 1, \ldots, n$$

Suppose now that we have discretized the curves, the error at the *j*-th point reads:

$$e_{i,j}(\boldsymbol{\theta}) \;=\; y_i^{exp}(t_j, \boldsymbol{d}_i) \;-\; f(t_j, \boldsymbol{d}_i, \boldsymbol{\theta}) \qquad , \quad j \in \mathcal{T}_i$$

We seek a set of parameters $\boldsymbol{\theta}_\alpha$ such that the related simulated curve overpredicts a given fraction α of experimental points, i.e. such that a fraction α of errors are positive and a fraction $(1-\alpha)$ are negative.

The simulated curve $f(t, \boldsymbol{d}, \boldsymbol{\theta}_\alpha)$ is referred to as an α - quantile curve.

Quantile regression (Koenker & Bassett, 1978)

It is shown that vector $\boldsymbol{\theta}_\alpha$ can be obtained by solving the following minimization probem:

$$\widehat{\boldsymbol{\theta}}_\alpha = \arg\min_{\boldsymbol{\theta}\in\mathbb{R}^p} \left(\sum_{i,j} \left(\alpha \langle e_{i,j}(\boldsymbol{\theta}) \rangle_+ + (1-\alpha) \langle e_{i,j}(\boldsymbol{\theta}) \rangle_- \right) \right)$$

where $\langle u \rangle_+ = \max(0, u)$ and $\langle u \rangle_- = -\min(0, u)$.

This problem is similar to a least absolute deviation scheme with weights α and $(1-\alpha)$ associated with the positive and negative errors, respectively.

It can be solved using an interior-point scheme (Koenker & Bassett, 1996) or a majoration-minimization (MM) algorithm (Hunter & Lange, 2000).

Asymmetric least squares (Efron, 1991)

It is possible to determine a vector $\widehat{\boldsymbol{\theta}}_w$ associated with a given weight w in order to construct a quantile curve. We have to solve:

$$\widehat{\boldsymbol{\theta}}_w = \arg\min_{\boldsymbol{\theta}\in\mathbb{R}^p} \left(\sum_{i,j} \left(w \langle e_{i,j}(\boldsymbol{\theta}) \rangle_+^2 + \langle e_{i,j}(\boldsymbol{\theta}) \rangle_-^2 \right) \right)$$

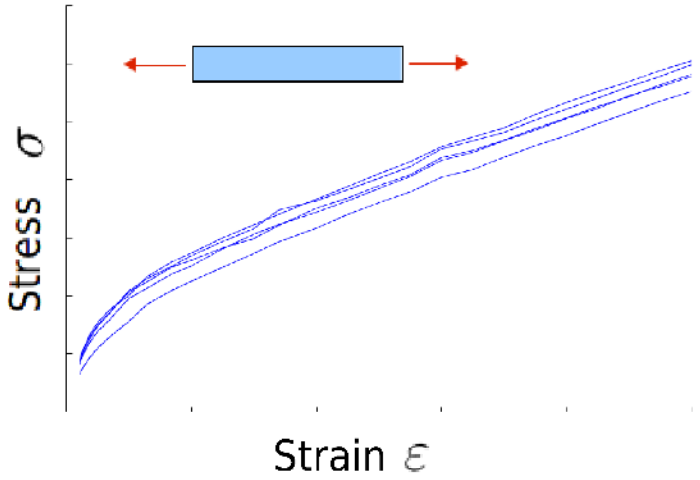
It is similar to a L2-type minimization problem with a specific weighting of the positive errors. A solving scheme can be simply implemented upon slightly modifying classical schemes (e.g. Levenberg-Marquardt).

Drawback. The weight w cannot be directly related to the prescribed quantile level α. We propose to find the suitable weight by dichotomy.

316LN steel under monotonic tensile loading (1)

316LN is a stainless steel which reveals resistant to corrosion and creeping at high temperatures. Its great ductility makes it resistant to crack propagation.

5 monotonic uniaxial tensile tests were carried out by EDF and AREVA, hence n=5 experimental curves.



Hardening model (Ramberg-Osgood)

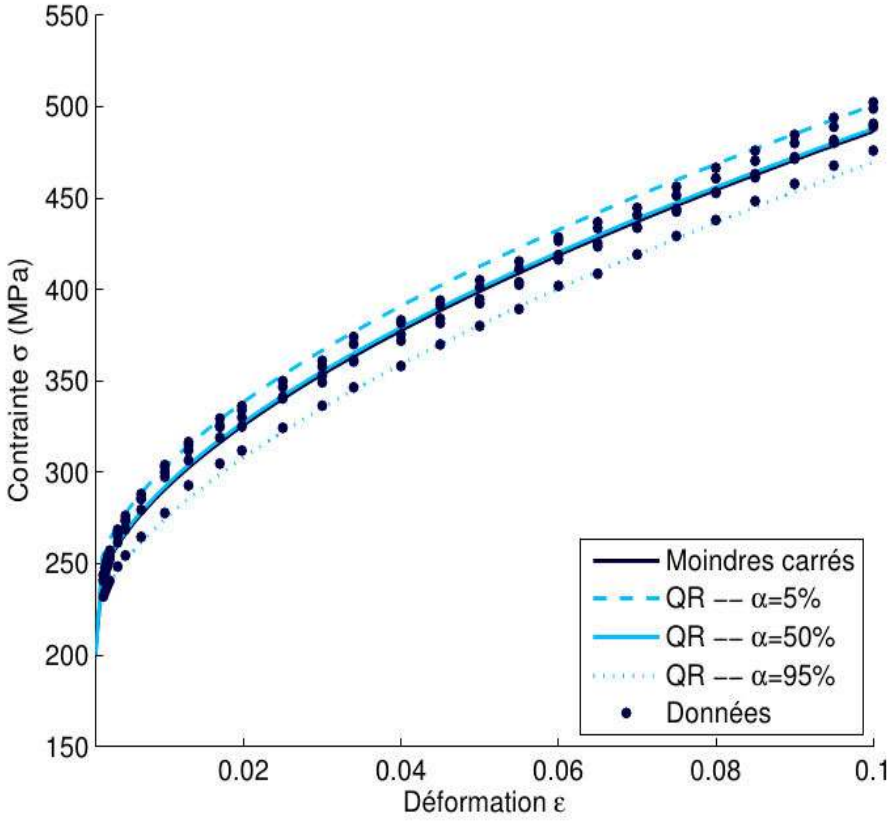
$$\sigma = f(\varepsilon, \boldsymbol{\theta}) = \sigma_y + k \left(\varepsilon - \frac{\sigma_y}{E}\right)^{1/m}$$

Parameters to calibrate:

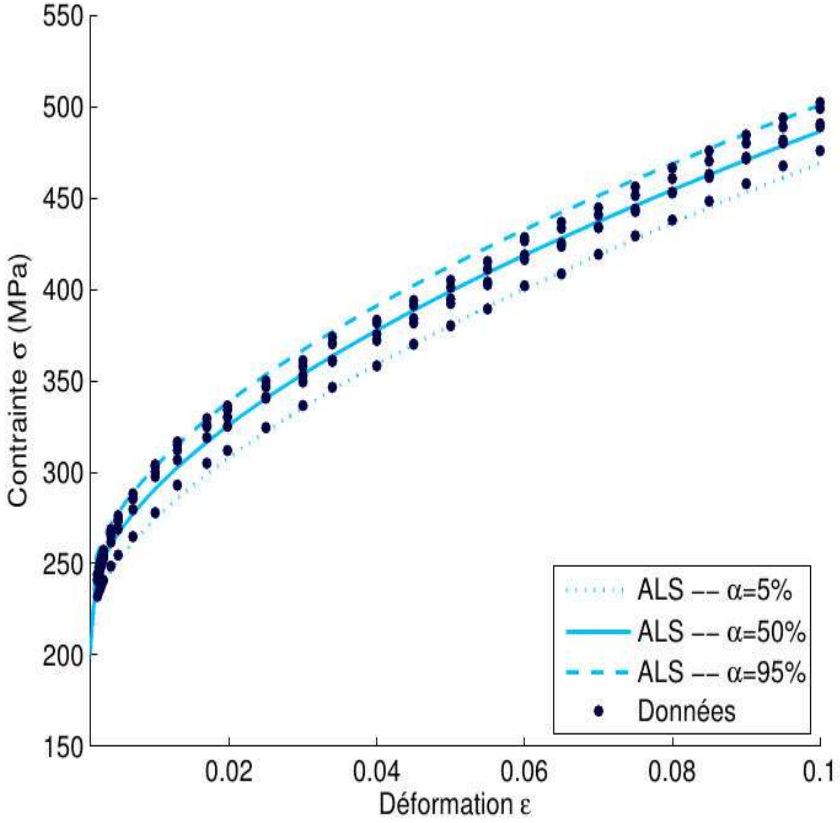
$$\boldsymbol{\theta} = \{\sigma_y, k, m\}$$

Results

QR



ALS



304L steel under cyclic tensile loading

Constitutive model (Chaboche-type model with prehardening)

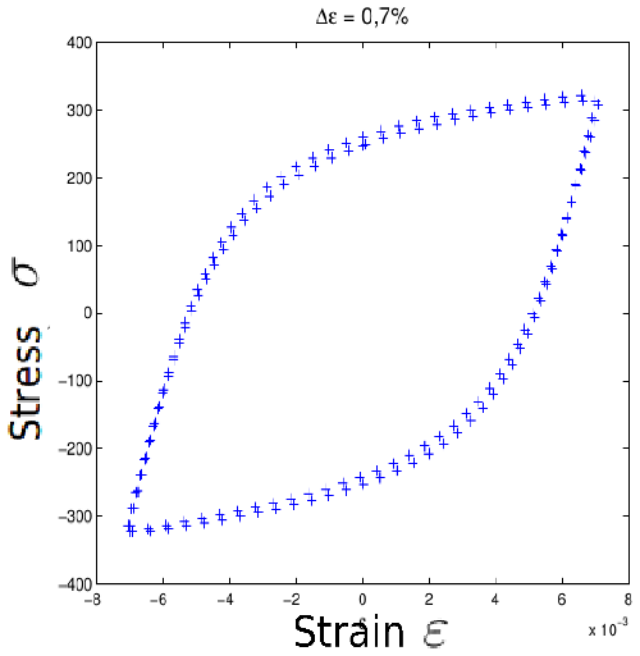
A set of *p*=6 parameters has to be calibrated:

- The Young's modulus: E
- 4 parameters related to the kinematic hardening: $C_1,\ C_2,\ \gamma_1^0,\ \gamma_2^0$
- The radius at the stabilized state of the plastic yield surface: k

Hence $\boldsymbol{\theta} = \{E, C_1, C_2, \gamma_1^0, \gamma_2^0, k\}$.

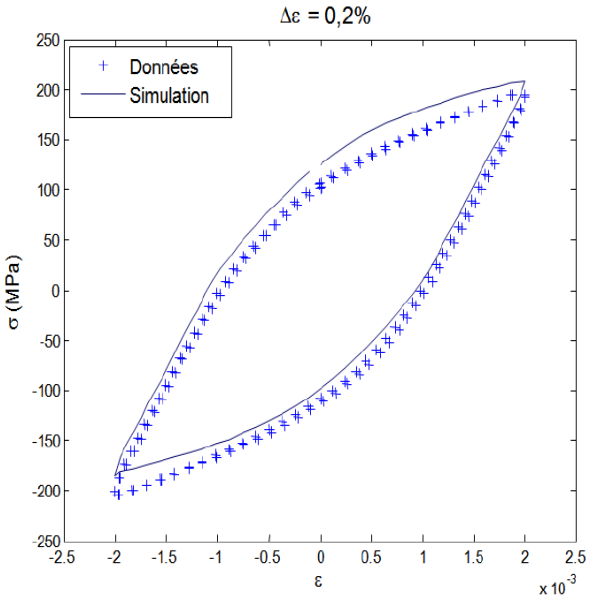
Experimental data (Cyclic tests)

4 levels of strain magnitude were considered. For each level, 2 cyclic tests were performed, hence a total of *n*=8 experimental curves.



Definition of a suitable model output

Problem. Overpredicting a given amount of data will *not* lead to a pessimistic or optimistic simulated curve in the case of cyclic tests. Hence applying quantile regression to the strain is not relevant.



Solution. We define a more appropriate model output, namely the elementary strain energy:

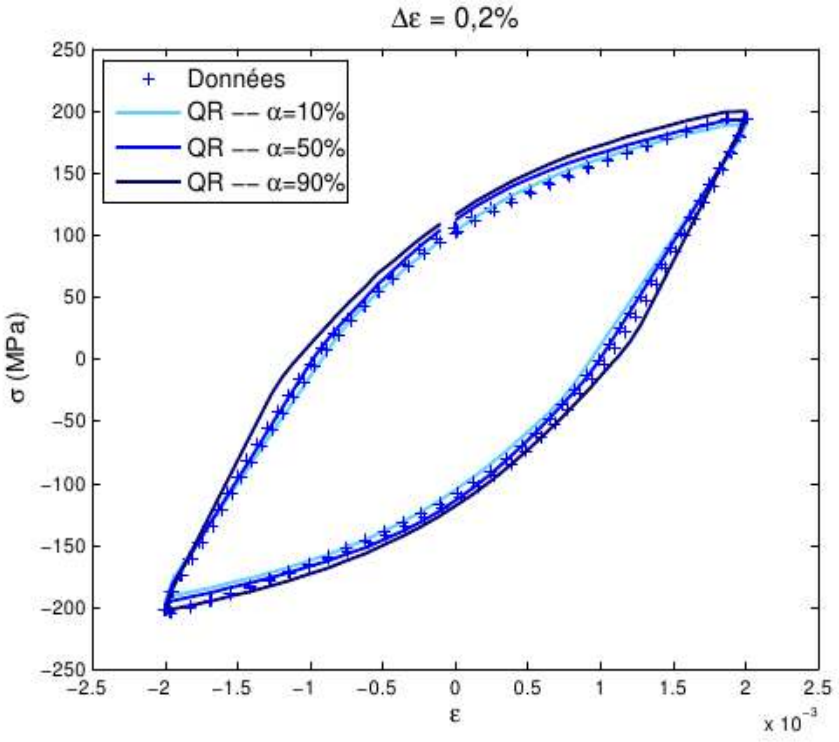
$$f(t, \boldsymbol{d}, \boldsymbol{\theta}) \;=\; \sigma(t)\;\delta\varepsilon(t)$$

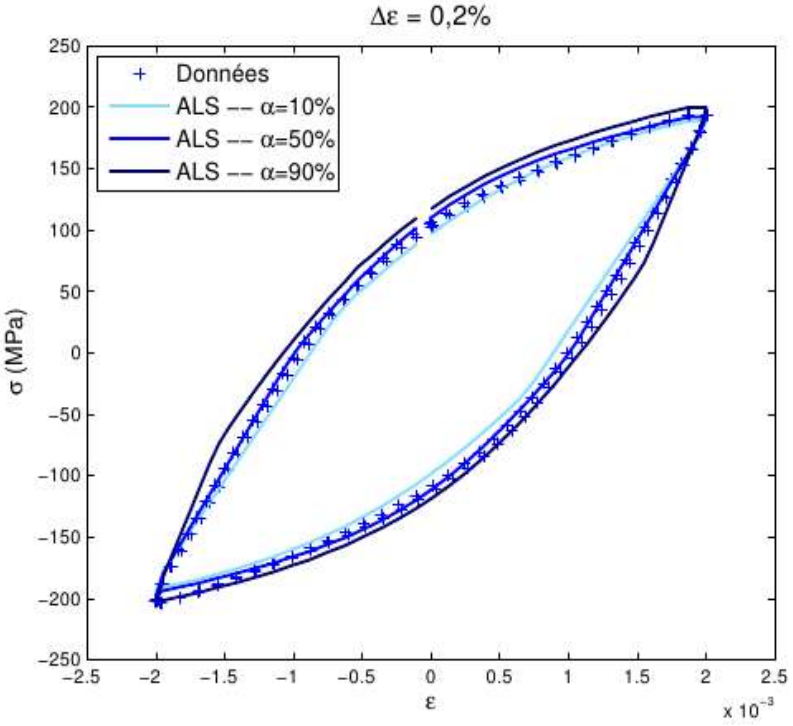
This way quantile regression will provide an « optimistic » curve which will contain the data and a « pessimistic » one which will be included in the data.

Quantile Regression applied to 3 data curves (1)

We only consider the curves related to the 3 lowest loading levels ($\Delta\varepsilon$ = 0,2% ; 0,3% ; 0,5%), hence n=6.

Results for the 0,2%-strain level (QR vs. ALS)





Quantile Regression applied to 3 data curves (2)

	α	E (MPa)	C_1 (MPa)	C_2 (MPa)	γ_1^0	γ_2^0	k	Prop. (%)	Cost
	10%	172 436	141 630	39 003	3 186	351	49	16	257
QR	50%	187 204	202 039	42 395	3 993	359	42	51	150
	90%	230 408	151 621	35 747	2 178	297	30	82	268
	10%	165 890	122 818	33 677	2 450	303	51	10	52
ALS	50%	189 292	192 750	41 242	3 491	359	37	50	78
	90%	273 062	184 757	36 604	2 012	280	3	91	224

Specific sets of constitutive parameters

- ALS leads to an ammount of overpredicted data that is closer to the prescribed level α than QR. Indeed the ALS stopping criterion depends directly on this ammount of points, whereas the QR one depends on a distance.
- QR requires more evaluations of the model than ALS in this example.

3. Probabilistic model calibration

Purpose of probabilistic calibration

Reminder: We have very few data and almost no prior knowledge on the constitutive parameters.

So we cannot infer a probabilistic model with the aim of predicting new experimental curves.

We will rather seek a probabilistic model that allows the simulations to properly « cover » the experimental data (e.g., the 95% reponse prediction band should border all the data points).

Regression-type model

We might be tempted to use a regression model of the form:

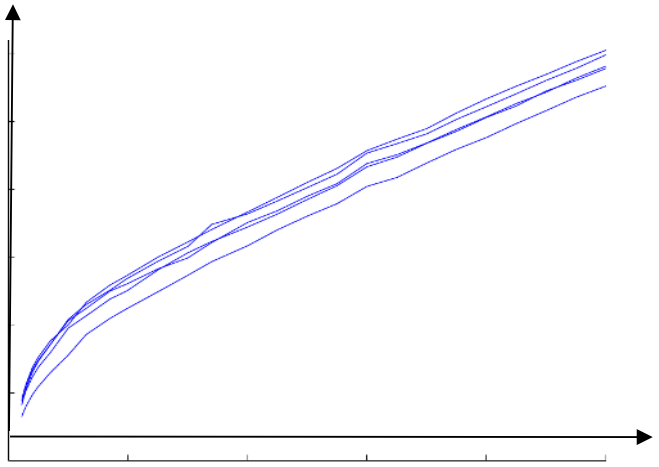
$$Y^{exp}(t) = f(t, \boldsymbol{\theta}) + \mathrm{Err}(t)$$

Deterministic but unknown material model

Zero-mean random error

This would allow us to derive statistical moments on the best estimate using standard assumptions.

However this regression model is not relevant, since the various curves do not seem to be affected by a (even possibly autocorrelated) random noise.



Assumption of a random material

Each test specimen is associated with a specific set of constitutive parameters $\boldsymbol{\theta}_i$. In this setup, the experimental scattering is partially due to a material dispersion. Hence the $\boldsymbol{\theta}_i$ are assumed to be realizations of a random vector $\boldsymbol{\Theta}$.

This leads to the following probabilistic model:

$$\mathsf{Y}^{exp}(t) \;=\; f(t,\boldsymbol{\Theta}) \;+\; \mathsf{Err}^{mod}(t) \;+\; \mathsf{Err}^{mes}(t)$$

Assumption. The model and measurement errors are supposed to be negligible compared to the material dispersion. Hence the previous equation reduces to:

$$\boxed{\mathsf{Y}^{exp}(t) \;=\; f(t,\boldsymbol{\Theta})}$$

Probabilistic calibration

Objective. Find a satisfactory joint PDF for Θ with respect to the observed data.

Constraints. (1) We have almost no prior knowledge on the parameters and (2) there are few observations.

(1) implies that we cannot use an informative Bayesian approach.

(2) implies that many common continuous distributions should not be rejected by statistical tests. So we can select the simplest distribution, that is a multivariate normal joint PDF.

Its parameters (mean values, variances and correlation coefficients) will be estimated by maximum likelihood.

Solving procedure

Let us consider *n* experimental curves and a parametric model $f(t, \boldsymbol{\theta})$.

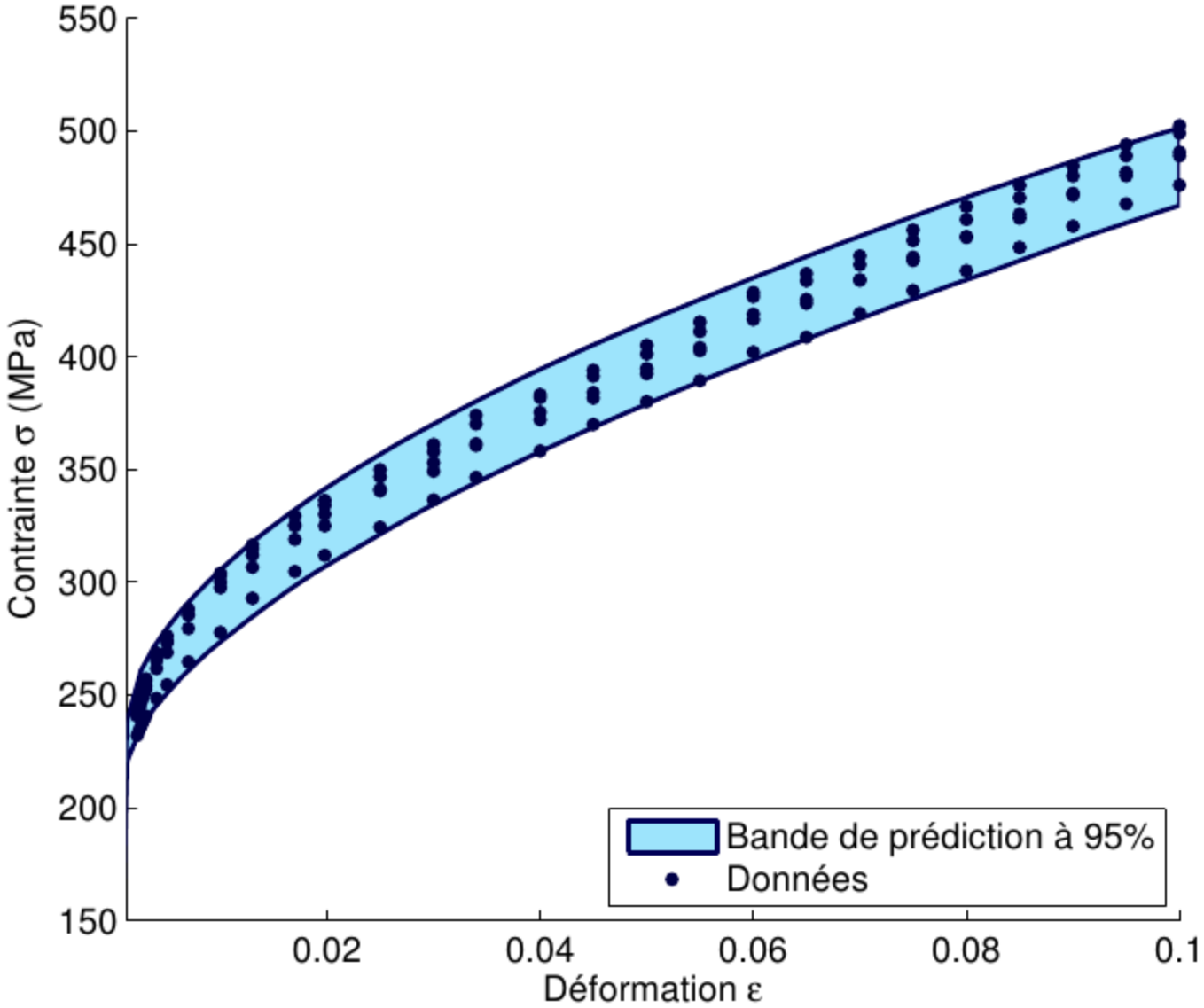
1. For *i*=1,...,*n*, find the vector of parameters $\widehat{\boldsymbol{\theta}}_i$ that minimizes the mean squared prediction error of the *i*-th curve (curve-by-curve calibration).

2. Set the hyperparameters of $\boldsymbol{\Theta}$ equal to the corresponding empirical statistics of the sample $\{\widehat{\boldsymbol{\theta}}_1, \ldots, \widehat{\boldsymbol{\theta}}_n\}$ (means, standard deviations and correlation coefficients).

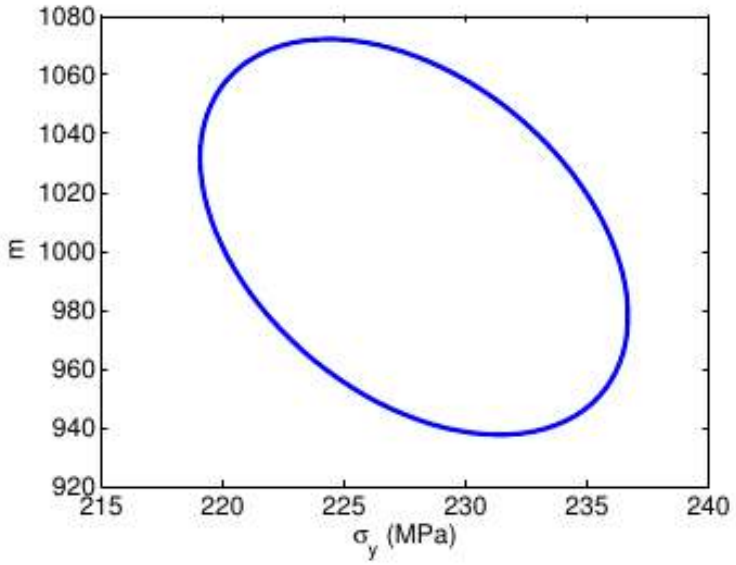
3. Generate a large sample (say, of size *N*=1000) of the estimated normal random vector, and evaluate the constitutive model at this point set. This yields a large set of simulated curves.

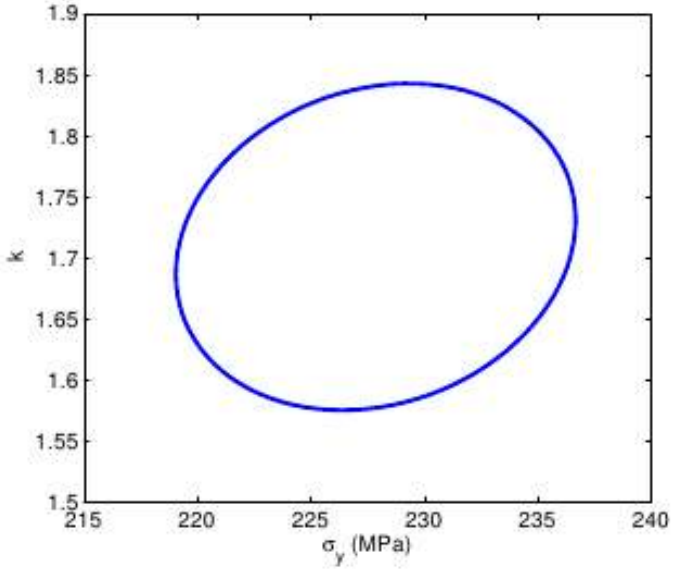
4. Construct a pointwise prediction band by computing empirical quantiles of the simulated curves at various instants.

Results for 316LN steel (1)

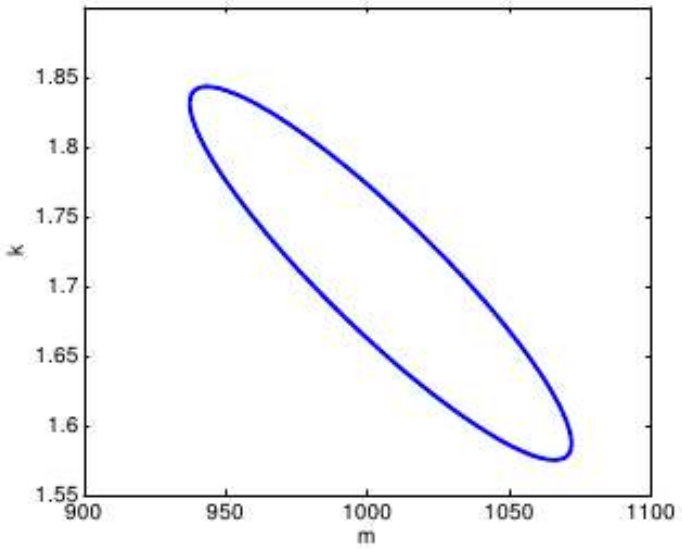


Results for 316LN steel (2)

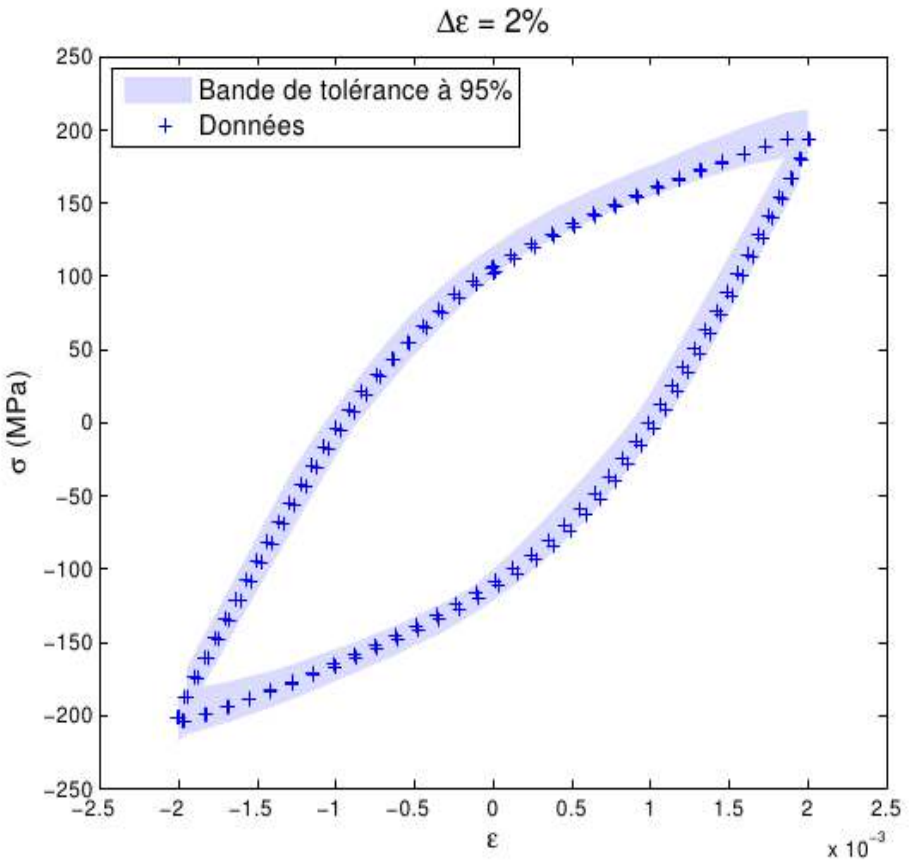


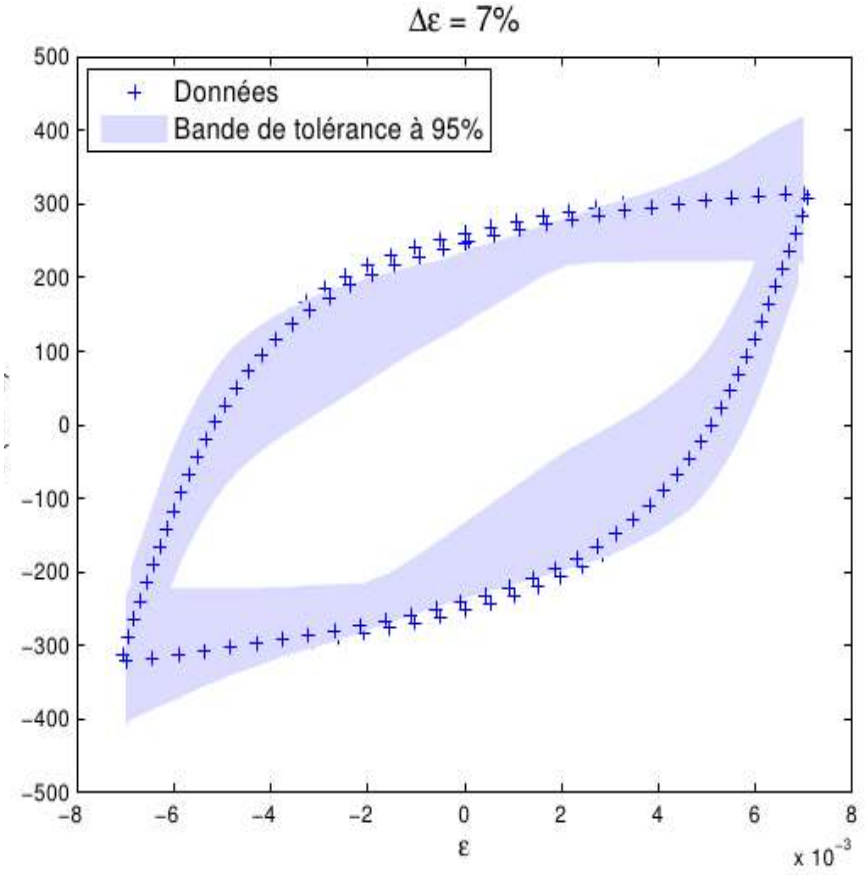


Parameters 95%-prediction ellipses



Results for 304L steel (1)



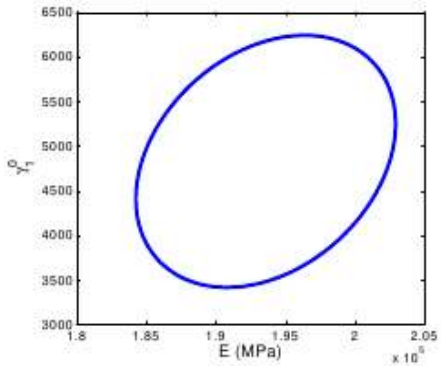


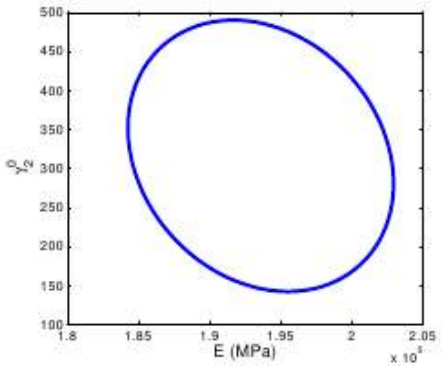
Results for 304L steel (2)

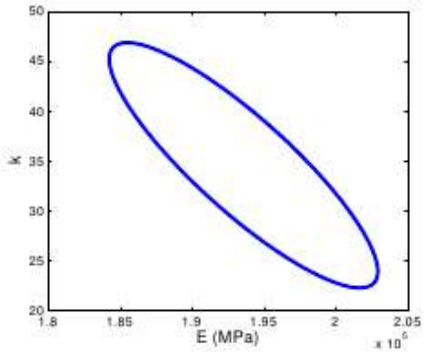
Univariate statistics

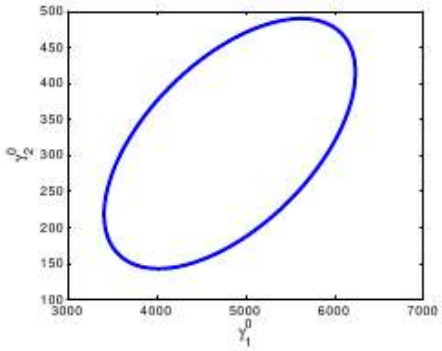
	E (MPa)	C_1 (MPa)	C_2 (MPa)	γ_1^0	γ_2^0	k
Moyennes	193 595	257 073	46 642	4 827	316	35
Coef. Var. (%)	3,9	15,0	16,3	23,9	45,0	29,1
Bornes inf. à 95%	188 307	230 318	41 358	4 026	217	28
Bornes sup. à 95%	198 884	283 829	51 926	5 627	414	41

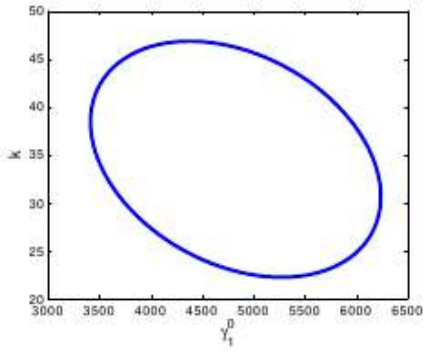
Results for 304L steel (3)

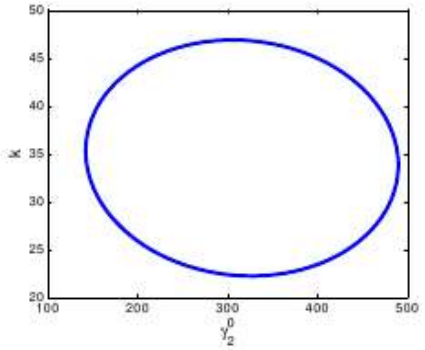












Parameters 95%-prediction ellipses

Summary

- Two types of methods were proposed:
  - Quantile regression to determine specific sets of parameters corresponding to envelope curves. It will allow the analyt to construct an interval of a (component) mechanical model at the cost of two deterministic calculations.
  - Curve-by-curve calibration to construct a simple probabilistic model of the parameters. This will make it possible to perform uncertainty and sensitivity analysis.

	Quantile Reg.	Curve-by-curve
Uncertainty analysis	-	+
Cost - constitutive model	+	+
Cost - macro mechanical model	++	-
Robustness – small samples	+	-

Outlook

- Curve-by-curve approach: make use of sparse covariance matrix estimation methods to deal with the case $n<p$

- Derive sensitivity measures in order to guide the identification process of a mechanical constitutive law:
  - Given an allowed number of tests, determine experimental conditions that should maximize the accuracy of the parameters estimates
  - In a purpose of material identification, find relevant tests in order to activate the various constitutive parameters
  - Extend a constitutive model to new environment/loading conditions

Thank you for your attention!

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Prediction error

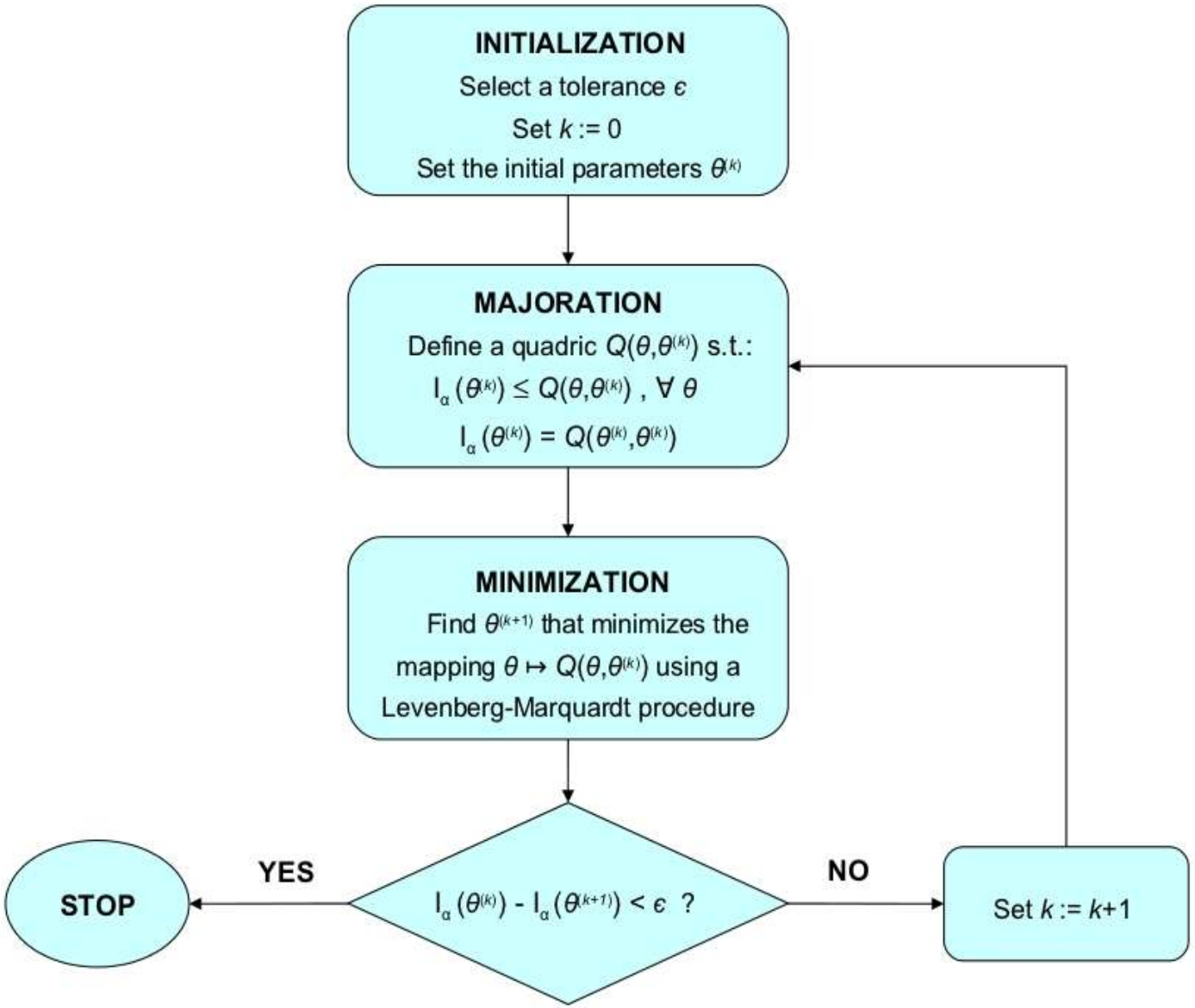
Decomposition of the prediction error:

$$Err_i(t) = h(t, \boldsymbol{d}, \boldsymbol{\theta}_i, \boldsymbol{\lambda}_i) - f(t, \boldsymbol{d}, \boldsymbol{\theta}_i) + f(t, \boldsymbol{d}, \boldsymbol{\theta}_i) - f(t, \boldsymbol{d}, \boldsymbol{\theta}) + Err_i^{mes}(t)$$

$$h(t, \boldsymbol{d}, \boldsymbol{\theta}_i, \boldsymbol{\lambda}_i) - f(t, \boldsymbol{d}, \boldsymbol{\theta}_i) \leftrightarrow Err_i^{mod}(t)$$

$$f(t, \boldsymbol{d}, \boldsymbol{\theta}_i) - f(t, \boldsymbol{d}, \boldsymbol{\theta}) \leftrightarrow Err_i^{mat}(t)$$

MM algorithm (Hunter & Lange, 2000)



Iterative asymmetric least squares