Modeling of the plastic mechanical response of soil-mixing materials: FFT-based computations and supervised learning

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Introduction

- Slides contain text so that the presentation can be read by people not attending the workshop.

Introduction

1. Introduction

Soil-Mixing materials

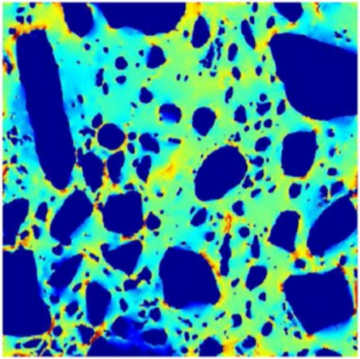
Figure 1 – Material sample, 177x103cm, 2.9kg, from Univ. Eiffel. Sampled from the ground-truth material in Loire. credit : Univ. Eiffel

- Soil-Mixing used to build seawall.
- Mix of in situ soil (from Loire) with binder (e.g. cement), to reduce permeability.
- In situ soil contains rock and mud, hence the material is composed of 3 phases.
- Plasticity implies a localization of the mechanical strain, hence an important effect of the microstructure, which we aim to study.

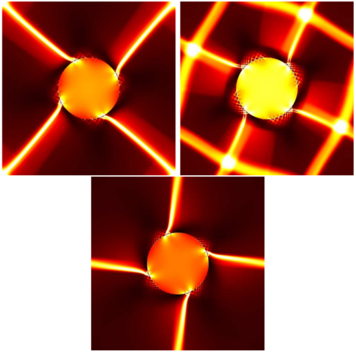
References

- Van Lysebetten, G., Vervoort, A., Maertens, J. and Huybrechts, N., 2014. Discrete element modeling for the study of the effect of soft inclusions on the behavior of soil mix material. Computers and Geotechnics, 55, pp.342-351

Plasticity and localization



(a) Elastic response (tensor C)
credit : F. Willot



(b) Image : plastic response, localization behavior with Von Mises criterion
credit : F. Willot

Segmented 3D image of the sample

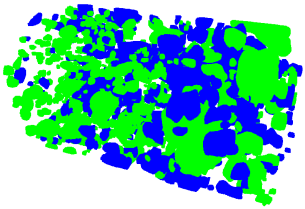


Figure 3 –
green : rock
blue : mud
cement : transparent

- Sample was sliced to get 3D data about the material.
- A 3D segmented image was created using this data.
- This image will be used in numerical computations.

Model of plasticity

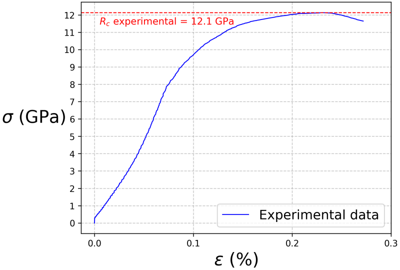


Figure 4 – Experimental simple compression curve, sample material. The local plasticity behavior is very complex but can be represented by a Mohr-Coulomb-type plasticity behavior.

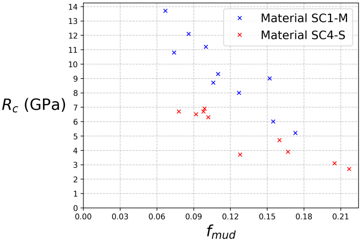


Figure 5 – Plasticity threshold R_c against volumetric fraction of mud. We see that depending on the material, the yield stress varies differently according to inclusions volumetric fractions.

Goal

- We want to predict the plasticity behavior of the material. We choose the plasticity threshold R_c to easily represent the macro-mechanical plasticity behavior. Hence, we want to predict the scalar value R_c.
- This yield stress depends on the volumetric fractions of mud and rocks, and on the binding material. Hence, we will have to choose numerical values for the parameters governing the mechanical behavior of the 3 phases to compute the yield stress.
- We will also have to choose simple features encapsulating the material's mechanical properties to make the predictions.

Plan

1. Modelisation of the material's local response with a plastic law with Mohr-Coulomb yield criterion, using full-field numerical computations carried out with Fast Fourrier transform algorithm.
2. Prediction of the effective yield stress R_c using the medium's overall response in the linear elastic regime with supervised learning.

1. Modelisation of the material's local response with a plastic law with Mohr-Coulomb yield criterion, using full-field numerical computations carried out with Fast Fourrier transform algorithm

Configuration studied

- A compression is easier to implement in a lab than a traction, hence compression is simulated to compare the results with Univ. Eiffel lab's results.
- In the lab, the compression along the xx axis is performed. Hence we compute the compression of the ground truth material along the xx axis.
- The material is compressed until it becomes plastic. We need to define a criterion for the material to become plastic. As stated in introduction, we choose the Mohr-Coulomb criterion.

Plasticity model

- The Mohr-Coulomb model gives a numerical criterion for the material to become plastic.
- This criterion is based on the values of the stress in the 3 mains directions :
  $f = \frac{1}{2}(\sigma_{max} - \sigma_{min}) + \frac{1}{2}(\sigma_{max} + \sigma_{min}) sin\Phi - ccos(\Phi)$
- See *Gomar, M., Goodarznia, I. and Shadizadeh, S.R., 2014. International Journal of Rock Mechanics Mining Sciences.*

Mohr Coulomb criterion

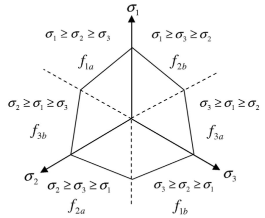


Fig. 2. Mohr–Coulomb surfaces

$$f = \frac{1}{2}(\sigma_{\max} - \sigma_{\min}) + \frac{1}{2}(\sigma_{\max} + \sigma_{\min})\sin\phi - c\cos\phi \qquad (76)$$

Figure 6 – With the Mohr-Coulomb model, a material remains elastic as long as its representation in the 3D stress field is inside the volume represented. Once the surface is reached, the material becomes plastic, and its representation in the strain field can go in any direction as long as it stays on the Mohr-Coulomb surface. The phenomenon is therefore highly non linear, and supposedly hard to predict.

Material properties

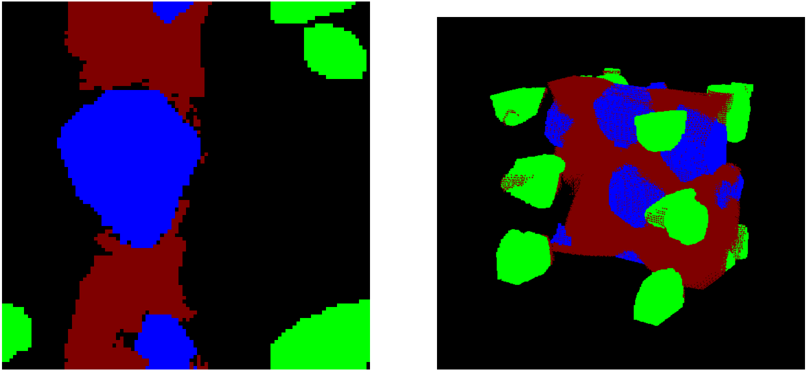
- Properties of the material must be supplied because they influence the mechanical behavior.
- Values of the Young modulus E, cohesion coefficient C, friction angle ϕ and Poisson coefficient ν are provided by Univ. Eiffel. We see that mud has a lower Young modulus, hence we except higher strain through mud.
- The cohesion coefficient of the matrix is unknown and obtained using exponential regression by Juba Amroui.

Phase	E (GPa)	Cohesion C (MPa)	Friction angle ϕ (°)	Poisson coefficient ν
Matrix	15.1	10	34	0.25
Mud	0.2	0.02	34	0.4
Rocks	75	30	40	0.25

Algorithm's parameters

- The deformation σ is gradually incremented with a fixed step, a fixed number of times.
- This loading step and the number of steps are determined experimentally, so that the strain σ has converged at the end of the experiment.

Images of the response on cubic microstructures



(a) (b)

Figure 7 – Cross section (a) and 3D image of a cubic microstructure (b), with thresholded strain field ϵ_{xx} in red, going through mud as expected.

Results of the computation on the ground-truth material

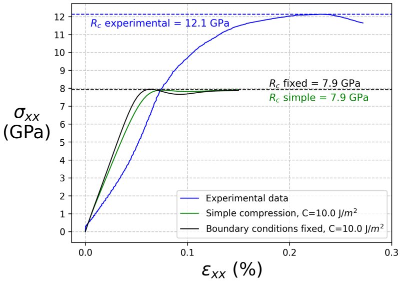


Figure 8 – Compression curves
Blue : Experimental data
Green : Numerical simple compression
Black : Boundary conditions fixed

We observe a factor two between the plasticity threshold from numerical and experimental data. It probably stems from the mechanical parameters of the material. In particular, the cohesion of the binding (matrix) material was obtained using exponential regression, which is proned to error. The difference in the shape of the numerical and experimental slopes probably stems from fractures inside the real-world material.

Explaining the discrepancy : mechanical parameters

- As explained in the introduction, mechanical parameters are used to make the computations.
- One of the parameters, the cohesion of the homogeneous matrix (binding) material C_{matrix}, was obtained using exponential regression with experimental data from heterogeneous material. This type of regression is prone to errors, hence C_{matrix} might be incorrect.
- We show with one numerical example that increasing C_{matrix} increases R_c. Hence, numerical curves could match experimental curves using inverse method on C_{matrix}, and potentially other parameters whose values are not necessarily correct for our material.

Results with increased C_{matrix}

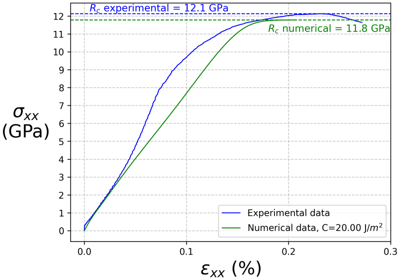
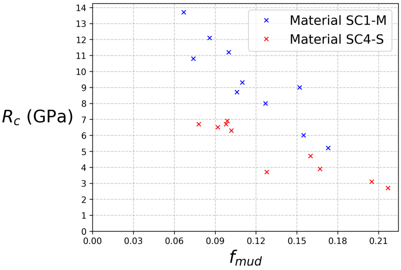


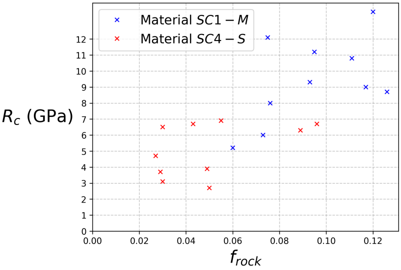
Figure 9 – Numerical and experimental strain-deformation curves close to one-another

- After increasing C_{matrix}, the numerical plasticity threshold is closer to the experimental one.
- Initial linear slopes match each other at the beginning. The experimental curve rapidly deviates from a strictly linear behavior because of fractures inside of the ground-truth material. The fractures are closed by the compression process, which reduces the deformation.

Inverse method to estimate C_{matrix} : experimental volumetric fractions impact on R_c



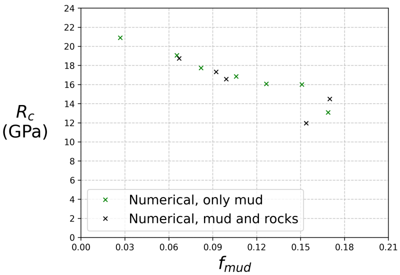
(a) R_c again f_{mud}



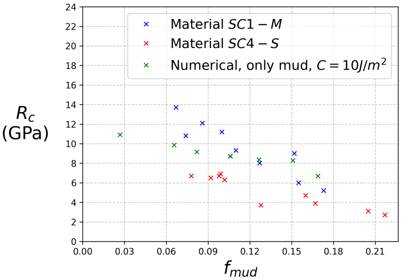
(b) R_c against f_{rock}

Figure 10 – R_c is positively correlated with f_{mud} and negatively with f_{rock}. The correlation is much better with f_{mud}.
Hence the exponential regression to find $R_c^{matrix}(f=0)$ was computed using f_{mud}.

Inverse method using numerical results



(a) R_c again f_{mud} for material with and without rocks



(b) R_c against f_{mud}

Figure 11 – Figure 11a shows that for numerical computations, the relation between f_{mud} and R_c is faintly influenced by f_{rock}. Hence we take $f_{rock} = 0$ for next numerical computations.
R_c and the slope are underestimated with $C = 10J/m^2$.

Numerical and experimental inverse method

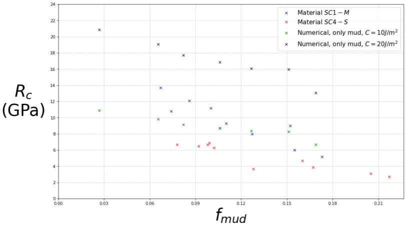


Figure 12 – Numerical and experimental impact of volumetric fraction of mud on R_c

- Increasing C_{matrix} to $20J/m^2$ leads to an overestimation of R_c for the numerical computations.
- C_{matrix} doesn't seem to influence much the slope.
- We conclude that the other parameters from the literature should be fine-tuned to match the experimental results.

Predictions

- Prediction of the effective yield stress Rc using the medium's overall response in the linear elastic regime with supervised learning.

Dataset

- Dataset of 3.000 100^3 random cubic microstructures, with predefined number of inclusions was generated.
- These microstructures have fixed boundary conditions, however the experiment on the ground-truth material showed that R_c is invariable according to boundary conditions. We assume that results with this configuration would be similar in the case of simple compression.

Results of numerical computations on random materials

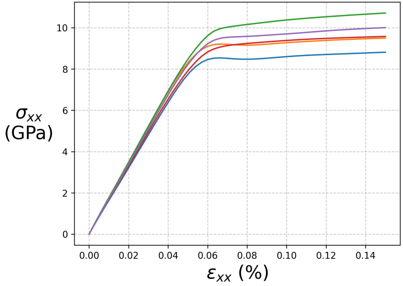


Figure 13 – 5 strain deformation curves

- We observe different slopes for the linear part of the strain - deformation curves.
- The plastic behavior is also different, as examplified by the overlapping red and orange curves.
- It stems from different localizations of inclusions and different volumetric fractions of mud and rock.
- We want to predict the plasticity threshold (constant part of the curve).

Prediction of plasticity threshold

- We need to find easy-to-compute features to make the predictions.
- It is very easy to get the young modulus of a material, because only one point is required.
- Hence, we suggest using the linear behavior of the material to predict the non linear plasticity threshold.
- We except a strong correlation between E_{xx} and R_c, as the plot suggests. However, the non-linear part of the curve should be influenced by E in other dimensions as well, because some curves have similar initial slope E_{xx} but different R_c.

Using the elasticity matrix C as feature

With some conditions (verified by our computation method not recalled here), the Hook law yields :

$$< \sigma_{ij} >= C_{ij,kl} < \epsilon_{kl} > \qquad (1)$$

$$\begin{pmatrix} < \sigma_{xx} > \\ < \sigma_{yy} > \\ < \sigma_{zz} > \\ < \sigma_{yz} > \\ < \sigma_{xz} > \\ < \sigma_{xy} > \end{pmatrix} = \begin{pmatrix} C_{11} & \dots & C_{16} \\ \vdots & \ddots & \vdots \\ C_{16} & \dots & C_{66} \end{pmatrix} \begin{pmatrix} < \epsilon_{xx} > \\ < \epsilon_{yy} > \\ < \epsilon_{zz} > \\ < 2\epsilon_{yz} > \\ < 2\epsilon_{xz} > \\ < 2\epsilon_{xy} > \end{pmatrix} \qquad (2)$$

The elasticity matrix encapsulates the linera behavior of the material and will be used to make the predictions.

Learning procedure

- Elasticity matrices C and plasticity thresholds R_c are computed for the 3.000 microstructures of the dataset.
- Features are all scalar and are normalized (0 mean, 1 variance) before making the predictions. This makes the prediction independant from the scale (e.g. E_{xx} will be bigger than the other matrix coefficients but not when it's normalized : its bigger value then doesn't impact its importance on the predictions).
- A linear regressor and multilayer-perceptron are trained using 80% (2400) of the microstructures.
- R^2 scores are computed using 20% of the dataset (600 microstructures).
- R^2 varies from 0 to 1, best regression having R^2 closer to 1.

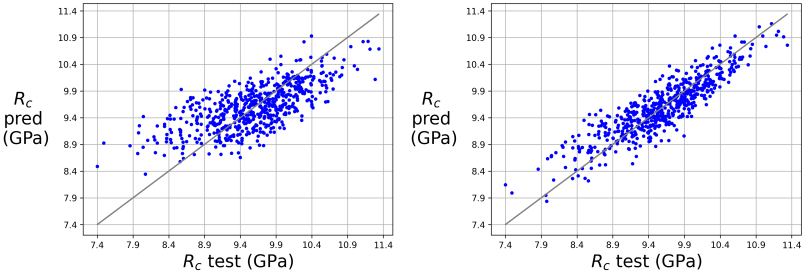
Impact of features on linear regression

Features	C_{11}	f_2, f_3	f_2, f_3, C_{11}	f_2, f_3, C
Number of features	1	2	3	23
Train R^2	0.464	0.482	0.663	0.7760
Test R^2	0.479	0.475	0.651	0.7763

Table 1 – Linear regression results

The table shows a good correlation between C_{11} (E_{xx}) and R_c.
We see that volumetric fractions are also correlated to R_c, but are not sufficient to make accurate predictions.
Combining both leads to better results.
Adding the whole linear matrix C improves even more the results, as expected.

Linear regression prediction results



(a) Only C_{11} as feature
$R^2_{test} = 0.48$

(b) f_{rock}, f_{mud}, C as features
$R^2_{test} = 0.78$

Figure 14 – R_c against R_c predicted for the test data.
Adding more linear features improves the predictions.

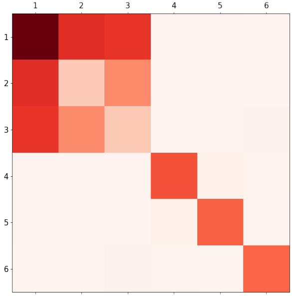
Multilayer Perceptron (MLP) results : similar to linear regression

Phase	Activation function	Number of hidden layers	Perceptron per hidden layer	Score
Grid-Search	ReLu ; logistic ; tanh ; identity	{2,3}	{8}	0.777
Test	logistic	2	(3,6)	0.778

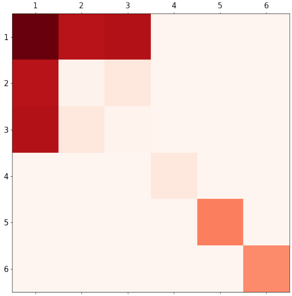
Table 2 – MLP hyperparameters and scores during the grid-search and the validation phases

Predictions with MLPs are similar to that with linear regressions, and are not presented here.

Elasticity matrices' coefficients importance



(a) Linear regression



(b) MLP

Figure 15 – Coefficient importance on the prediction is similar for both the MLP and the linear regression predictors.

Interpretation of the prediction results

- As expected, $C_{11} = E_{xx}$ is the most important coefficient in the prediction.
- Only the theoretically non-zero coefficients of the elasticity matrix have an importance on the results. These coefficients are close to zero in the simulation (around $e - 15$), however because of the normalization, they could influence the simulation. As the compression is along the xx axis, we can show with symmetry and statistical arguments that these coefficients cannot have any importance on the simulation results.

Conclusion

- We modelled the plastic mechanical response of soil-mixing materials using FFT-based computations, comparing our simulation results with experimental data.
- We used the medium's overall response in the linear elastic regime to predict the effective yield stress, and showed improved predictions when all elastic modes are used in the predictions.
- Our results can be linked with non linear homogenization theories which make use of the elastic response to predict the non-linear behavior.
- Many more features could be taken to make predictions : elastic response in the other axes, covariances, minimal surfaces...