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Gaussian process emulation for rapid in-plane mechanical homogenization of periodic masonry

LUIS C. M. da Silva [1, a *], ANDRÉ Jesus[2,b] and GABRIELE Milani[1,c]

[1] Department of Architecture, Built environment and Construction engineering (A.B.C.), Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133, Milan, Italy

[2] School of Architecture, Building and Civil Engineering, Loughborough University, Leicestershire, England, United Kingdom

[a]luiscarlos.martinsdasilva@polimi.it, [b]a.jesus@lboro.ac.uk, [c]gabriele.milani@polimi.it

*corresponding author

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Abstract. Numerical homogenization strategies can provide average mechanical responses, either in stress or coupled-stress quantities, which include many phenomenological features. Nonetheless, a direct application of numerical homogenization in sensitivity analysis in which uncertainty is propagated becomes impractical, as hundreds or thousands of simulations are conventionally required. In this study, a reliable and rapid predictive surrogate model is developed aiming to characterize the homogenized response of masonry. The case of English-bond arrangement is addressed, and the following steps are considered: (1) creation of a synthetic database through numerical homogenization based on a Finite-Element method, generated by randomization of model parameters; (2) training of a nonlinear Gaussian process; and (3) approximation of homogenized stress-strain curves for a masonry wall and for both linear and nonlinear ranges. The performance of the proposed technique is evaluated using training-validation-test in terms of computational accuracy. Results indicate that computational time is lessened 1200% while relative errors remain below 5-10%.

Introduction

Including uncertainty in the mechanical analysis of masonry structures is generally achieved through forward propagation of uncertainty. Input variables are assumed to be random and uncertainty is propagated aiming to evaluate its effect in the mechanical response [1]. Inverse propagation is the opposite process and it is receiving attention due to the advance of surrogate modelling, as for instance to predict cement mortar strength [2], but also in dynamic identification problems [3]–[5]. Inverse problems allow predicting the parameters of a given system through a data-driven framework and within a probabilistic prediction interval. Although these are receiving a growing attention [6], its extension to the mechanical analysis of masonry structures is still limited.

In such a context, the present study tries to tackle such opportunity. Classical Finite-Element (FE) and Discrete-Element (DE) strategies are expensive to run when analyzing masonry structures in the inelastic range and when parameter uncertainty is considered. This study addresses such difficulty by reducing the high computational time-cost required. The provision of a mesoscopic numerical model through a homogenization technique [7]–[11] and within a probabilistic framework has a paramount role, as it can provide data for training and testing of a surrogate model. In specific, a Gaussian process [12] is adopted since it offers promising accuracy when applied to non-linear structural mechanics problems [6], [13]. The presented strategy is thus based on numerical tools only, which is convenient as it precludes the need of other data sources such experimental tests. Hence, the study develops a simple-to-use and fast model based on a

Gaussian process to predict the homogenized in-plane mechanical response of an English-bond masonry wall.

Mesoscopic boundary value problem

A meso-mechanical problem is solved to compute average field variables for the in-plane mechanical response of masonry. The problem is formulated for the case of regular and periodic masonries. A single Representative Volume Element Ω_m (RVE) is defined. The kinematical description of the in-plane case assumes that the macroscopic strain tensor E is obtained as the volume average of the mesoscopic strain field $\epsilon_m = \epsilon_m(y)$ over the associated volume V_m of the RVE (Eq. (1)). The mesoscopic strain field can be decomposed into a macro-scale and meso-scale contributions. The homogenized generalized stress is computed considering the mesoscopic stress field $\boldsymbol{\sigma}_m$ upon RVE equilibrium following the Hill-Mandell principle. The homogeneous macroscopic stress tensor $\boldsymbol{\Sigma}$ can be written as the volume average of the mesoscopic stress field $\boldsymbol{\sigma}_m = \boldsymbol{\sigma}_m(y)$ over the RVE (Eq. (1)).

$$E = \frac{1}{V_m}\int_{\Omega_m} \epsilon_m \, dV \quad , \quad \boldsymbol{\Sigma} = \frac{1}{V_m}\int_{\Omega_m} \boldsymbol{\sigma}_m \, d\Omega \ . \tag{1}$$

A 2D unit-cell FE model based on a Kirchhoff-plate theory method is adopted to solve the meso-scale BVP. Brick units ($235 \times 115 \times 70$ mm^3) are modelled as elastic and through quadrilateral FEs and material nonlinearity is lumped on mortar joints that are represented through interface FEs. Such assumption is particularly adequate for strong unit masonry structures [14]. The so-called composite interface model [15] is adopted, which is able to reproduce fracture, frictional slip and crushing along the interface elements of the joints. It is defined by a convex composite yield criterion with three individual functions able to represent softening behavior, i.e. a (i) a tension cut-off criterion designated as $f_{criterion,1}$ and defined in Eq. (3); (ii) a Mohr-Coulomb shear criterion designated as $f_{criterion,2}$ and defined in Eq. (4); and (iii) a cap in compression designated as $f_{criterion,3}$ and defined in Eq. (5).

$$f_{criterion,1}(\boldsymbol{\sigma}, k_1) = \sigma - \bar{\sigma}_1(\mathrm{k}_1) \quad and \quad \bar{\sigma}_1 = f_t \, \mathrm{e}^{\left(-\frac{f_t}{G_{ft}^{I}} k_1\right)} \ . \tag{3}$$

$$f_{criterion,2}(\boldsymbol{\sigma}, k_2) = |\,\tau\,| + \sigma \tan(\phi)(\mathrm{k}_2) - \bar{\sigma}_s(k_2) \quad and \quad \bar{\sigma}_2 = c \, \mathrm{e}^{\left(-\frac{c}{G_{ft}^{II}} k_2\right)} \ . \tag{4}$$

$$f_{criterion,3}(\boldsymbol{\sigma}, k_3) = \frac{1}{2}\left(\boldsymbol{\sigma}^T \mathbf{P} \boldsymbol{\sigma}\right) + \mathbf{p}^T \boldsymbol{\sigma} - \bar{\sigma}_3^2(k_3) \ . \tag{5}$$

Here, $\boldsymbol{\sigma}$ is the generalized stresses, f_t is the interface bond strength, c is the interface cohesion, ϕ is the friction angle; $\mathbf{P}$ is a projection diagonal matrix and $\mathbf{p}$ a projection vector based on material parameters [15]; G_{ft}^{f}, G_f^{II} are the mode-I and mode-II fracture energy terms, respectively; $\bar{\sigma}_1$, $\bar{\sigma}_2$ and $\bar{\sigma}_3$ are the effective stresses of each the adopted yield functions governed by the internal scalar variables κ_1, κ_2 and κ_3, respectively. The deterministic strategy given in [14] was enriched by attributing probability distribution functions to each input parameter; specifically to both geometric and material properties. If X defines the random input variables X_i, then one can write the following:

$$X = \{E_{brick}\, , E_{mortar}\, , f_t\, , G_{ft}^{I}\, , f_c\, , G_{fc}^{I}\, , c\, , G_f^{II}\, , f_c\, , t_{joint}\, , t\} \ . \tag{6}$$

in which $\forall X_i \in X : X_i = f(x)$ whereas $f(x)$ is assumed to be an uniform function. The sampling of random variables (RVs) is achieved by the Latin Hypercube method. The solution of the mesoscopic BVP is processed N_{simul} times, hence finding N_{simul} homogenized quantities.

Gaussian process emulation

A Gaussian process is a non-parametric probabilistic model that can be used for nonlinear regression of an existent model, hence approximating the structural response containing noise for classification problems [16]. For the present study, the nonlinear mapping between the input parameters and the corresponding homogenized stress-strain curves of the masonry will be approximated using a G_p. A G_p is fully defined by a mean and covariance function that is dependent on a set of parameters – known as hyperparameters – that must be estimated from a training data set. The mean *m* and covariance *V* are given by:

$$m(x) = \mathbf{H}(x)\boldsymbol{\beta} \qquad V(x,x) = s^2\mathbf{R}(x,x) . \tag{7}$$

in which $\mathbf{H} \in \mathsf{R}^{N\times p}$ is a regression matrix, $\boldsymbol{\beta} \in \mathbb{R}^p$ is a vector of regression coefficients, x represents the strain and parameters described in the previous section that define the stress-strain curve, s^2 is a scalar response variance and $\mathbf{R} \in \mathbb{R}^{N\times N}$ is a correlation matrix. The matrix $\mathbf{H}$ contains N first order polynomial functions $h_1(x) = [1\, x_1]$ of degree $p = 2$. The matrix $\mathbf{R}$ contains the entries for a correlation function, which has been assumed to be linear:

$$R(\omega, x, x') = \max\{0, 1 - \omega\,|\,x - x'\,|\} . \tag{8}$$

in which ω is a roughness parameter [17] that represents how roughly the response changes between training data points. The hyperparameters that define the above functions, $\vartheta = \{\boldsymbol{\beta}, s^2, \boldsymbol{\omega}\}$, must be estimated from training data. Summarily, a likelihood function that describes how well the model fits the data is established and maximized. To simplify it, analytical expressions can be found for s^2 and $\boldsymbol{\beta}$. For further theoretical details see [16].

Training and testing data

The homogenized $\Sigma - E$ curves have been generated through the meso-mechanical model. The input parameters are given in Table 1. Both friction angle ϕ and masonry wall thickness t are assumed to be deterministic variables. An elastic response has been considered in compression, which is acceptable for a strong-unit-weak-joint type of masonry.

Table 1 – Random input for the meso-mechanical model.

	Random parameters						
X_i	E_{brick} (N/mm^2)	E_{mortar} (N/mm^2)	$f_{t,mortar}$ (N/mm^2)	G_{ft}^{I} (N/mm)	G_{f}^{II} (N/mm)	c (N/mm^2)	t_{joint} (mm)
$E[X_i]$	[1000;15000]	[500;4000]	[0.05;0.40]	[0.005;0.015]	[0.02;0.055]	[0.05;0.80]	[10;15]

The generated data comprises 2697 curves for each associated Cauchy's deformation mode: (i) in-plane tension xx, (ii) in-plane tension yy, and (iii) in-plane shear xy. Homogenized curves are presented in Fig. 1. Each curve is composed of 100 points with a total of $N_{samples} = 269700$ points. Nonetheless, only 2.9% have been randomly selected for the training ($N_{training} = 7600$ points) and 20% for the testing ($N_{testing}$).

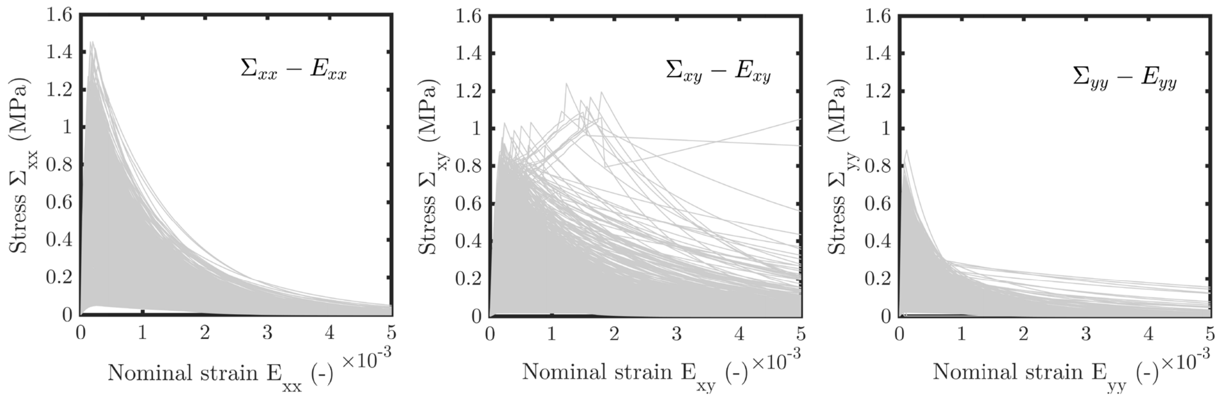
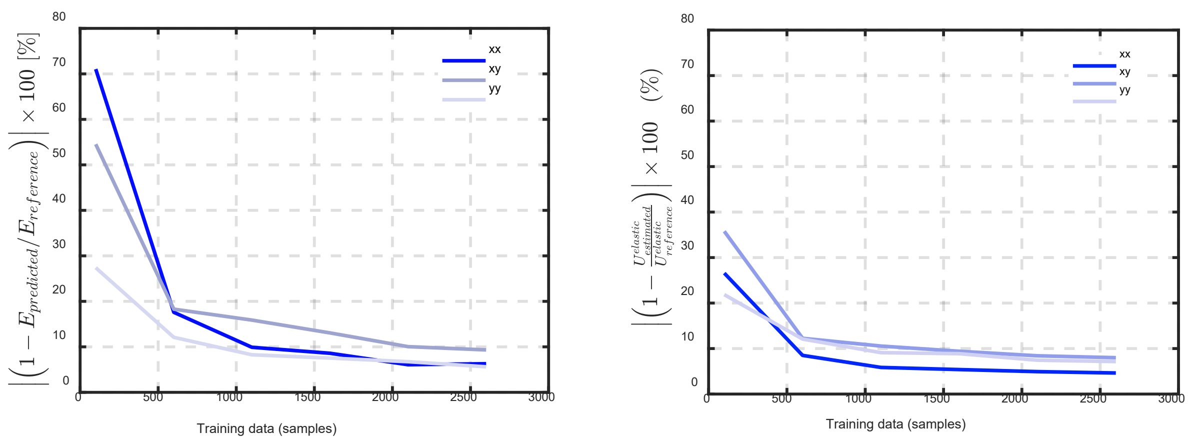


Fig. 1 – Probabilistic homogenized stress-strain curves used in the Gaussian process emulation.

Discussion of results

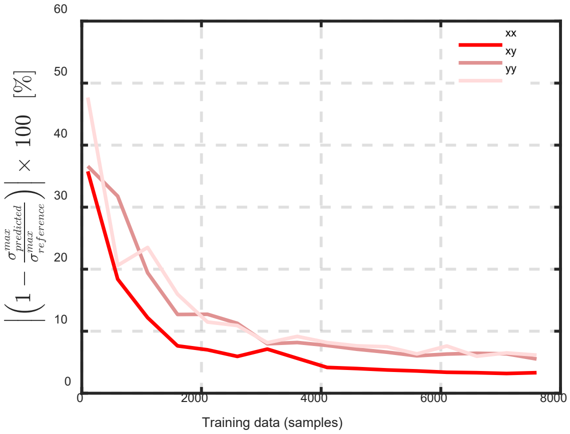
The elastic and inelastic homogenized responses have been emulated separately since the curves have a discontinuity between these ranges. Note that such division is easily achieved by scanning the peak of each curve. The mean function and prediction interval of two curves are hence predicted – elastic and inelastic ranges –, being subsequently merged to form the full predicted in-plane response of the periodic masonry arrangement. The mean function is used for the validation or testing of the predicted results. In the elastic part, both the estimated Young's modulus and elastic strain energy are validated against the reference data, as given in Fig. 2. Results indicate that relative errors below 10% are expected for the homogenized Young's modulus when the training data are equal to 2697 points. From an energetic standpoint, a total of 1500 points are enough to respect such threshold of 10%, as given in Fig.2(b).



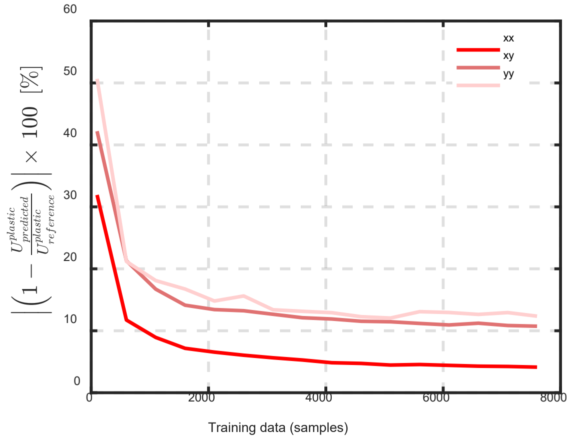
(a) Young's modulus (b) elastic strain energy

Fig. 2 – Relative errors of the predicted response in the elastic range.

For the inelastic range, the estimated peak and plastic strain energy, based on the Gp predicted mean function, are evaluated and compared with the reference testing data. The relative error is plotted in Fig. 3(a) and Fig. 3(b), respectively. In this case, all the training samples ($N_{training}$ = 7900 points) have been used, for which relative errors below 5% for the peak stress are found; and around 10% for the plastic strain energy in shear (xy curve) and vertical tension (yy curve) and around 4% for horizontal tension (curve xx). We can also highlight the existence of a plateau for $N_{training}$ > 7900 points, meaning that the improvement of the solution accuracy in the inelastic range may require a significant number of more data.



(a) peak stress



(b) plastic strain energy

Fig. 3 – Relative errors of the predicted response in the inelastic range.

Conclusions

A Gaussian process has been used to predict the in-plane mechanical homogenized response of an English-bond masonry. The framework is purely numerical data-driven and proved its efficiency to compute the elastic and inelastic ranges of the in-plane tension (horizontal and vertical directions) and shear responses has been demonstrated. The homogenized Young's modulus, the elastic strain energy, the strength value, and the inelastic strain energy were considered to demonstrate the accuracy level. Generally, the Gaussian process is effective and accurate even for a small number of training data. After the training step, it requires in average 4 seconds to compute each homogenized curve, i.e. ~1200% lower than the time required by the meso-mechanical simulation. Its generalizability is guaranteed, as the topological input is independent on the type of masonry bond. Lastly, the study gives an important contribution to the application of inverse methods for the structural analysis of masonry structures. The results are promising and may lead to a future publication, in which case studies at a structural level will be provided.

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