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Stochastic modeling of a class of stored energy functions for incompressible hyperelastic materials with uncertainties

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Abstract

In this Note, we address the construction of a class of stochastic Ogden's stored energy functions associated with incompressible hyperelastic materials. The methodology relies on the maximum entropy principle, which is formulated under constraints arising in part from existence theorems in nonlinear elasticity. More specifically, constraints related to both polyconvexity and consistency with linearized elasticity are considered and potentially coupled with a constraint on the mean function. Two parametric probabilistic models are thus derived for the isotropic case and rely in part on a conditioning with respect to the random shear modulus. Monte Carlo simulations involving classical (e.g. Neo-Hookean or Mooney-Rivlin) stored energy functions are then performed in order to illustrate some capabilities of the probabilistic models. An inverse calibration involving experimental results is finally presented.

Résumé

Sur une classe de potentiels élastiques stochastiques pour les matériaux hyperélastiques incompressibles isotropes. Dans cette Note, on s'intéresse à la construction d'une classe de modèles stochastiques pour des matériaux hyperélastiques incompressibles. La méthodologie de construction repose sur le principe du maximum d'entropie, formulé à partir de contraintes induites par les théorèmes d'existence en élasticité non-linéaire. Plus précisément, des contraintes associées à la polyconvexité et à la cohérence avec l'élasticité linéarisée sont introduites, et éventuellement couplées avec une contrainte relative à la fonction moyenne. Deux modèles probabilistes paramétriques pour les densités d'énergie considérées sont par suite proposés dans le cas isotrope, et reposent notamment sur un conditionnement vis-à-vis du module de cisaillement aléatoire. Des simulations numériques de Monte Carlo pour des potentiels classiques (e.g. Néo-Hookéen ou Mooney-Rivlin) sont ensuite conduites afin d'illustrer les capacités du modèle. Une identification inverse basée sur des résultats expérimentaux est enfin présentée.

Key words: Maximum entropy principle; stochastic modeling; hyperelasticity; stored energy functions; polyconvexity; uncertainties.

Mots- $cl\acute{e}s$: Principe du maximum d'entropie; modélisation stochastique; hyperélasticité; densités d'énergie élastiques; polyconvexité; incertitudes.

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1. Introduction

In this work, we address the construction of parametric probabilistic representations for stored energy functions defining incompressible hyperelastic materials. Such models are dedicated to predictive modeling in nonlinear elasticity, where engineered or biological materials can exhibit uncertainties (at some scale of interest) that are worth taking into account. This random behavior may arise from e.g. batch-to-batch variability or processing defects for manufactured composites, or from intrinsic variability in the case of complex heterogeneous materials (see [1] and the references therein for a discussion regarding experimental results in biomechanics, for instance). Unlike the linear case, where the modeling and propagation of uncertainties gave rise to an extensive literature (both in applied mathematics and computational mechanics; see the references below), the nonlinear case has surprisingly received little attention – at least, from a modeling standpoint. Uncertainty propagation from microscale to macroscale was analytically addressed in [2], where bounds on effective properties are expressed, by means of Hashin-Shtrikman bounds, in terms of the fluctuation terms. Computational multiscale frameworks based on a microscale description were further proposed in [3,4] and rely on the combination between interpolation schemes (in the space of macroscopic deformations) and polynomial chaos expansions [5]. The construction of relevant parametric probabilistic representations for stored energy functions exhibiting some uncertainties therefore remains an intricate and open question. In this paper, we propose a very first contribution to this field in the framework of Information Theory, and restrict the derivations to the isotropic case for the sake of readability. The aim is to develop a methodology for the derivation of relevant probabilistic models for stochastic stored energy functions, thanks to the principle of maximum entropy. In order to ensure mathematical consistency, the latter is formulated under constraints related to existence theorems in nonlinear elasticity and coherence at small strains. These constraints can be subsequently supplemented with an additional one associated with the mean function, if need be. The paper is organized as follows. For completeness, a brief review of hyperelasticity is first presented in section § 2. The construction of a class of stochastic stored energy functions for incompressible hyperelastic materials is then addressed in section § 3. Monte Carlo simulations and an inverse identification based on experimental data are finally presented in section § 4 in order to illustrate the model capabilities.

Notation. Throughout this paper, use will be made of the following matrix sets:

- (i) $\mathbb{M}_d(\mathbb{R})$ the set of real $(d \times d)$ matrices;
- (ii) $\mathbb{L}_d(\mathbb{R})$ the set of real $(d \times d)$ matrices with an unitary determinant.

Deterministic (resp. stochastic) scalar-valued random variables are denoted α or a (resp. α or A). Similarly, deterministic (resp. stochastic) vectors are denoted by \boldsymbol{a} (resp. \boldsymbol{A}).

2. Framework for deterministic hyperelasticity

Let $\Omega \subset \mathbb{R}^3$ be a bounded open connected set with a sufficiently regular boundary, and denote by $\overline{\Omega}$ its closure. It is assumed that Ω is occupied by a homogeneous incompressible isotropic hyperelastic material characterized by a stored energy function $\widehat{w} : \mathbb{L}_3(\mathbb{R}) \to \mathbb{R}$ such that [6,7,8,9]:

$$[\widehat{T}([F])] = \frac{\partial \widehat{w}([F])}{\partial [F]} - \widetilde{h}[F]^{-T}, \forall [F] \in \mathbb{L}_3(\mathbb{R}), \qquad (1)$$

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where $[\widehat{T}]: \mathbb{L}_3(\mathbb{R}) \to \mathbb{M}_3(\mathbb{R})$ is the response function associated with the first Piola-Kirchoff tensor $[T]: \overline{\Omega} \to \mathbb{M}_3(\mathbb{R}), [F]$ is the deformation gradient and \widetilde{h} is a Lagrange multiplier (which is typically interpreted as an hydrostatic pressure) enforcing the incompressibility condition. In addition to isotropy, the stored energy function is classically assumed to satisfy frame-invariance, so that according to representation theorems, there exists a function w such that:

$$\widehat{w}([F]) = w(v_1([F]), \ v_2([F]), \ v_3([F])) \ , \tag{2}$$

where $\{v_j([F])\}_{j=1}^3$ are the eigenvalues of [F]. Such a class of strain energy functions was extensively studied for natural rubbers and proposed, on the basis of phenomenological concerns, by Ogden [10,11]. More specifically, the following algebraic form was postulated [10]:

$$\widehat{w}([F]) = \sum_{i=1}^{m} \alpha_i \Phi_{\gamma_i}([F]) + \sum_{j=1}^{n} \beta_j \Upsilon_{\delta_j}([F]) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) ,$$
(3)

where $\{\alpha_i, \gamma_i\}_{i=1}^m$ and $\{\beta_j, \delta_j\}_{j=1}^n$ are sets of model parameters. In Eq. (3), $\Phi : \mathbb{L}_3(\mathbb{R}) \to \mathbb{R}$ and $\Upsilon : \mathbb{L}_3(\mathbb{R}) \to \mathbb{R}$ are the functions defined as

$$\Phi_{\gamma_i}([F]) = v_1([F])^{\gamma_i} + v_2([F])^{\gamma_i} + v_3([F])^{\gamma_i} - 3 \tag{4}$$

and

$$\Upsilon_{\delta_{i}}([F]) = (\upsilon_{1}([F])\upsilon_{2}([F]))^{\delta_{j}} + (\upsilon_{1}([F])\upsilon_{3}([F]))^{\delta_{j}} + (\upsilon_{2}([F])\upsilon_{3}([F]))^{\delta_{j}} - 3 \tag{5}$$

for any deformation gradient $[F] \in \mathbb{L}_3(\mathbb{R})$. The above stored energy density function can be shown to be polyconvex whenever the above parameters verify $\alpha_i > 0$ for $1 \le i \le m$, $\gamma_1 \ge \cdots \ge \gamma_m \ge 1$, $\beta_j > 0$ for $1 \le j \le n$ and $\delta_1 \ge \cdots \ge \delta_n \ge 1$. This polyconvexity property, together with suitable growth conditions, ensures the existence of minimizers for the total energy functional [12] (see also [13,7] for discussions). If $\gamma_1 \ge 2$ and $\delta_1 \ge 3/2$, the stored energy density function defined by Eq. (3) can be shown to exhibit a coercivity property which implies the existence of a global minimizer of the total energy function for pure displacement, pure traction and displacement-traction problems [14] (note that similar results exist for compressible materials; see [12,7]).

For m=n=1 and $\gamma_1=\delta_1=2$, the stored energy function under consideration reduces to the Mooney-Rivlin model for incompressible materials:

$$\widehat{w}([F]) = \alpha_1 \left(\|[F]\|^2 - 3 \right) + \beta_1 \left(\|\text{Cof}([F])\|^2 - 3 \right) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) , \tag{6}$$

where $\alpha_1 > 0$ and $\beta_1 > 0$ by the constraint of polyconvexity. The Neo-Hookean model for incompressible materials [15] can be recovered by disregarding the second term in the right-hand side of Eq. (3) and by setting m = 1 and $\gamma_1 = 2$:

$$\widehat{w}([F]) = \alpha_1 \left(\|[F]\|^2 - 3 \right) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) , \tag{7}$$

with $\alpha_1 = \mu/2 > 0$ by the consistency condition. Specific discussions on existence theorems for the Neo-Hookean model can be found in [12,16].

3. Stochastic models of stored energy functions for incompressible hyperelastic materials

3.1. Definition of a parametric probabilistic representation

Let \widehat{W} be the stochastic stored energy function corresponding to the probabilistic modeling of \widehat{w} , and let p and η be the vectors in \mathbb{R}^{n_p} such that

$$\mathbf{p} = (\alpha_1, \dots, \alpha_m, \beta_1, \dots, \beta_n) , \quad \mathbf{\eta} = (\gamma_1, \dots, \gamma_m, \delta_1, \dots, \delta_n) ,$$
 (8)

with $n_p := m + n$. In this work, it is assumed that the model exponents involved in \widehat{W} are deterministic (and may correspond to a fit with respect to a mean response function, for instance), whereas the remaining coefficients are modeled as statistically dependent random variables. Let P be the vector-valued random variable corresponding to the stochastic modeling of p and for which the probabilistic model is sought. The construction of the latter is performed by imposing that the stochastic stored energy function is:

- (i) polyconvex almost surely (a.s.), which follows whenever $0 < P_k$, $1 \le k \le n_p$, a.s.;
- (ii) coherent at small strains, meaning that P and η satisfy the usual consistency condition with linearized theory [8,9]:

$$\sum_{k=1}^{n_p} P_k \eta_k^2 = 2\mu , \qquad (9)$$

where μ is the random variable with values in $]0, +\infty[$ modeling the stochastic shear modulus, and

$$P_k < \frac{2\mu}{\eta_k^2} , \quad 1 \leqslant k \leqslant n_p \tag{10}$$

almost surely (recall that $\eta_k > 0$, $1 \le k \le n_p$, by construction). For an incompressible Mooney-Rivlin material, the above constraints reduce to $2(P_1 + P_2) = \mu$ and $0 < P_k < \mu/2$, $i \in \{1, 2\}$, as

Note that since the exponents are assumed to be deterministic, the coercivity property does not constraint the construction of the probabilistic model. From a methodological standpoint, and following Eqs. (9) and (10), a probabilistic model is first constructed for the random shear modulus μ , and the one related to \boldsymbol{P} is then derived through a conditioning on μ . In order to ensure that Eq. (9) holds a.s., an arbitrary component of \boldsymbol{P} , say P_{n_p} , is algebraically defined as

$$P_{n_p} = \frac{1}{\eta_{n_p}^2} \left\{ 2\mu - \sum_{k=1}^{n_q} P_k \eta_k^2 \right\} , \qquad (11)$$

so that the construction of the probabilistic model is achieved on the random vector $\mathbf{Q} := (P_1, \dots, P_{n_q})$ that takes its values in a subset of \mathbb{R}^{n_q} , with $n_q := n_p - 1$. Note here that the probabilistic models for \mathbf{Q} and \mathbf{p} completely define the system of marginal probability distributions for the stochastic process $\{\widehat{W}([F]), [F] \in \mathbb{L}_3(\mathbb{R})\}$. One is then concerned with the construction of the joint probability density function $p_{\mathbf{p},\mathbf{Q}}$ of random variables \mathbf{p} and \mathbf{Q} such that:

$$p_{\mathbf{p},\mathbf{Q}}(\mu,\mathbf{q}) = p_{\mathbf{p}}(\mu) \times p_{\mathbf{Q}|\mathbf{p}=\mu}(\mathbf{q}) . \tag{12}$$

Next, a normalized vector-valued random variable U is introduced and defined as

$$U_k := \left(\frac{\eta_k^2}{2\mu}\right) (Q_k | \mu = \mu) , \quad 1 \leqslant k \leqslant n_q , \qquad (13)$$

with $\mu > 0$ a.s. Hence

$$p_{\mathbf{Q}|\mu=\mu}(\mathbf{q}) = p_{\mathbf{U}}([G(\mu)]^{-1}\mathbf{q}) \times \frac{1}{(2\mu)^{n_q}} \prod_{k=1}^{n_q} \eta_k^2,$$
 (14)

where $[G(\mu)]$ is the invertible diagonal $(n_q \times n_q)$ matrix given by

$$[G(\mu)]_{kk} = \frac{2\mu}{\eta_k^2} , \quad 1 \leqslant k \leqslant n_q ,$$
 (15)

and

$$p_{\mu,Q}(\mu,q) = p_{\mu}(\mu) \times p_{U}([G(\mu)]^{-1}q) \times \frac{1}{(2\mu)^{n_q}} \prod_{k=1}^{n_q} \eta_k^2.$$
 (16)

It can be deduced from Eqs. (10), (11) and (13) that U takes its values in the interior of the n_q -dimensional simplex S, independent of the shear modulus, such that:

$$S := \left\{ \boldsymbol{u} \in \mathbb{R}^{n_q} \mid 0 < u_k < 1, \ 1 \leqslant k \leqslant n_q, \ 1 - \sum_{k=1}^{n_q} u_k > 0 \right\} . \tag{17}$$

Below, the explicit forms of p_{\parallel} and p_U are constructed in the framework of Information Theory and more precisely, by invoking the principle of maximum entropy (MaxEnt) [17,18,19]. The latter allows for the derivations of probability distributions that, while consistent with the information available on the random variables to be defined, maximize the uncertainties as measured by Shannon's differential entropy. Such an approach is therefore well suited in order to derive unbiased probabilistic models, and was fruitfully used so as to construct stochastic representations for tensor-valued random variables and random fields in linear elasticity [20,21,22,23]. To the best knowledge of the authors, this work is the first attempt to construct information-theoretic models in finite elasticity.

3.2. Stochastic modeling of the random shear modulus

It is assumed that random variable μ satisfies the following constraints:

$$\mathbb{E}\left\{ \mathbf{\mu}\right\} =\mu,\tag{18a}$$

$$\mathbb{E}\left\{\log(\mathbf{p})\right\} = \nu \ , \quad |\nu| < +\infty \ . \tag{18b}$$

The first constraint given by Eq. (18a) means that the mean value of μ is known, whereas the second one is a repulsive constraint implying that μ and μ^{-1} are both second-order random variables [24]. The MaxEnt based probability density function of random variable μ is then given by:

$$p_{\mu}(\mu) = \mathbb{1}_{\mathbb{R}_{+}^{*}}(\mu) \ k_0 \ \mu^{\rho_1 - 1} \ \exp\left(-\frac{\mu}{\rho_2}\right) \ , \quad \forall \mu > 0 \ ,$$
 (19)

where $\mathbb{1}_{\mathbb{R}_+^*}$ is the indicator function of \mathbb{R}_+^* , k_0 is the normalization constant and (ρ_1, ρ_2) is a set of strictly positive Lagrange multipliers raised by the MaxEnt principle. It can further be shown after little algebra that $(\rho_1, \rho_2) = (\delta_{\mathbb{p}}^{-2}, \underline{\mu} \, \delta_{\mathbb{p}}^2)$, with $\delta_{\mathbb{p}}$ and $\underline{\mu}$ the coefficient of variation and mean value of \mathbb{p} respectively, so that the above probability density function writes

$$p_{\mathbb{P}}(\mu) = \mathbb{1}_{\mathbb{R}_{+}^{*}}(\mu) \frac{\mu^{\delta_{\mathbb{P}}^{-2} - 1}}{(\mu \delta_{\mathbb{P}}^{2})^{\delta_{\mathbb{P}}^{-2}} \Gamma(\delta_{\mathbb{P}}^{-2})} \exp\left(-\frac{\mu}{\underline{\mu} \delta_{\mathbb{P}}^{2}}\right) , \quad \forall \mu > 0 ,$$
 (20)

where Γ is the Gamma function [25] defined as:

$$\Gamma(z) = \int_0^{+\infty} t^{z-1} \exp\left(-t\right) dt , \quad \forall z > 0 .$$
 (21)

It follows that under the constraints defined by Eqs. (18a) and (18b) (which correspond to the minimal mathematical requirements), the random shear modulus is a Gamma-distributed random variable with parameters $(\delta_{\mu}^{-2}, \mu \delta_{\mu}^2)$.

3.3. Construction of a probabilistic model under constraints related to polyconvexity and coherence at small strains

3.3.1. General derivations

Let us consider the following constraints on random variable U:

$$\mathbb{E}\left\{\log\left(U_k\right)\right\} = \nu_k, \quad 1 \leqslant k \leqslant n_q , \qquad (22a)$$

$$\mathbb{E}\left\{\log\left(1 - \sum_{k=1}^{n_q} U_k\right)\right\} = \nu_{n_p} , \qquad (22b)$$

where $|\nu_k| < +\infty$ for $1 \le k \le n_p$. These equality constraints are repulsive with respect to the boundaries of simplex S, thus insuring that U has values in S almost surely. Let $(1 - \lambda_1), \ldots, (1 - \lambda_{n_p})$ be the associated (n_p) Lagrange multipliers. It can then be shown that the probability density function p_U of U takes the form

$$p_{\boldsymbol{U}}(\boldsymbol{u}) = \mathbb{1}_{\mathcal{S}}(\boldsymbol{u}) \left\{ \frac{\Gamma\left(\sum_{k=1}^{n_p} \lambda_k\right)}{\prod_{k=1}^{n_p} \Gamma(\lambda_k)} \right\} \left(\prod_{k=1}^{n_q} u_k^{\lambda_k - 1}\right) \left(1 - \sum_{k=1}^{n_q} u_k\right)^{\lambda_{n_p} - 1}, \quad \forall \boldsymbol{u} \in \mathcal{S}.$$
 (23)

It follows that U is distributed according to a Dirichlet-type I distribution [26] with parameters $\lambda_1, \ldots, \lambda_{n_p}$. Whereas the integrability condition requires that the Lagrange multipliers are all strictly positive, the property $\lambda_k > 1$, $1 \leq k \leq n_p$, is further imposed in order to ensure unimodal first-order marginal probability functions, as well as proper repulsion conditions from the boundaries of S. Let \mathbb{D}_{λ} denote the admissible set for the vector-valued representation of the Lagrange multipliers:

$$\mathbb{D}_{\lambda} := \{ \lambda \in \mathbb{R}^{n_p} \mid \lambda_k > 1, \ 1 \leqslant k \leqslant n_p \} \ . \tag{24}$$

In addition, it can be deduced that each random variable U_k , $1 \le k \le n_q$, follows a beta-type I distribution with parameters $(\lambda_k, \ \xi_k)$, where $\xi_k := (\sum_{\ell=1}^{n_p} \lambda_\ell) - \lambda_k$, and

$$p_{U_k}(u) = \mathbb{1}_{[0;1[}(u) \left\{ \mathcal{B}(\lambda_k, \xi_k) \right\}^{-1} u^{\lambda_k - 1} (1 - u)^{\xi_k} , \quad \forall u \in]0, 1[,$$
 (25)

in which $\mathcal{B}: \mathbb{R}_+^* \times \mathbb{R}_+^* \to \mathbb{R}$ is the beta function given by [25]:

$$\mathcal{B}(x,y) = \int_0^1 t^{x-1} (1-t)^{y-1} dt.$$
 (26)

The following proposition can then be deduced from the above derivations.

Proposition 3.1 Let $\widehat{W}: \mathbb{L}_3(\mathbb{R}) \to \mathbb{R}$ be the stochastic stored energy function defined as

$$\widehat{W}([F]) := \sum_{i=1}^{m} Q_{i} | \mathbb{1} \Phi_{\gamma_{i}}([F]) + \sum_{j=1}^{n-1} Q_{m+j} | \mathbb{1} \Upsilon_{\delta_{j}}([F]) + \delta_{n}^{-2} \left(2\mathbb{1} - \sum_{k=1}^{n_{q}} Q_{k} | \mathbb{1} \eta_{k}^{2} \right) \Upsilon_{\delta_{n}}([F]) , \qquad (27)$$

for all $[F] \in \mathbb{L}_3(\mathbb{R})$, in which $n_q := m + n - 1$ and

- (1) $\gamma_1 \geqslant 2$ and $\gamma_1 \geqslant \ldots \gamma_m \geqslant 1$;
- (2) $\delta_1 \geqslant 3/2$ and $\delta_1 \geqslant \cdots \geqslant \delta_n \geqslant 1$;
- (3) the random shear modulus μ is a Gamma-distributed random variable with parameters $(\delta_{\mu}^{-2}, \underline{\mu} \, \delta_{\mu}^{2})$, in which μ and δ_{μ} are respectively the mean value and coefficient of variation of μ ;
- (4) the random variable $\mathbf{Q}|_{\mathbb{H}}$ is defined component-wise as $(Q_k|_{\mathbb{H}} = \mu) := 2\mu U_k \eta_k^{-2}$, $1 \leqslant k \leqslant n_q$, where the random variable \mathbf{U} takes its values in the interior of the n_q -dimensional simplex

$$S := \left\{ \mathbf{u} \in \mathbb{R}^{n_q} \mid 0 < u_k < 1, \ 1 \le k \le n_q, \ 1 - \sum_{k=1}^{n_q} u_k > 0 \right\}$$

and follows a Dirichlet-type I distribution with vector-valued parameter λ such that $\lambda_k > 1$ for $1 \leq k \leq n_p$.

Then, \widehat{W} is polyconvex, coherent at small strains and satisfies the coerciveness inequality almost surely.

The above proposition ensures that for the constructed class of stochastic stored energy function, there exists a global minimizer for the energy functional almost surely (which is a fundamental property). Finally, and from a practical standpoint, it is worth noticing that if Y_1, \ldots, Y_{n_p} are independent Gamma random variables with respective parameters $(\lambda_1, 1), \ldots, (\lambda_{n_p}, 1)$, then the random variable U such that

$$U_i := Y_i \times \left(\sum_{k=1}^{n_p} Y_k\right)^{-1} , \quad 1 \leqslant i \leqslant n_q , \qquad (28)$$

is distributed according to a Dirichlet-type 1 distribution with parameters $(\lambda_1, \ldots, \lambda_{n_p})$ (see Theorem 4.1, p. 594 in [27] for instance) – hence providing a very simple and robust generator for the random variable U involved in the above proposition.

3.3.2. Particular case of an incompressible Neo-Hookean material

For an incompressible isotropic Neo-Hookean material, the stochastic stored energy function then takes the following form:

$$\widehat{W}([F]) = \frac{\mathbb{I}}{2} \left(\|[F]\|^2 - 3 \right) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) , \tag{29}$$

in which μ is the Gamma-distributed random variable defined in section 3.2, with parameters $(\delta_{\mu}^{-2}, \mu \delta_{\mu}^{2})$.

3.3.3. Particular case of an incompressible Mooney-Rivlin material

In the case of an incompressible isotropic Mooney-Rivlin model (for which m = n = 1 and $\gamma_1 = \delta_1 = 2$), the stochastic stored energy function reduces to:

$$\widehat{W}([F]) = Q|\mu\left(\|[F]\|^2 - 3\right) + \left(\frac{\mu}{2} - Q|\mu\right)\left(\|\text{Cof}([F])\|^2 - 3\right) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) , \tag{30}$$

where $(Q|\mathfrak{p}=\mu):=\mu\,U/2$ and the random variable U follows a beta-type I distribution with parameters $\lambda_1>1$ and $\lambda_2>1$:

$$p_U(u) = \mathbb{1}_{\mathcal{S}}(u) \left\{ \mathcal{B}(\lambda_1, \lambda_2) \right\}^{-1} u^{\lambda_1 - 1} (1 - u)^{\lambda_2 - 1}, \quad \forall u \in \mathcal{S},$$
 (31)

with $\mathcal{S} =]0, 1[$.

3.4. Construction of a probabilistic model under constraints related to polyconvexity, coherence at small strains and mean values

3.4.1. General derivations

Here, the previous constraints are supplemented with constraints related to the mean values. More specifically, the probabilistic model is derived under the constraints given by Eqs. (22a)-(22b), as well as under the following algebraic constraint

$$\mathbb{E}\left\{\boldsymbol{U}\right\} = \underline{\boldsymbol{u}} \,\,\,(32)$$

related to the mean value of U. The probability density function p_U of U then takes the form:

$$p_{U}(\boldsymbol{u}) = \mathbb{1}_{\mathcal{S}}(\boldsymbol{u}) \ k_0 \left(\prod_{k=1}^{n_q} u_k^{\lambda_k - 1} \right) \left(1 - \sum_{k=1}^{n_q} u_k \right)^{\lambda_{n_p} - 1} \exp\left(- \sum_{k=1}^{n_q} \xi_k u_k \right) , \tag{33}$$

where S is the n_q -dimensional simplex defined by Eq. (17), k_0 is the normalization constant, $\{\lambda_k\}_{k=1}^{n_p}$ and $\{\xi_k\}_{k=1}^{n_q}$ are the sets of Lagrange multipliers associated with constraints given by Eqs. (22a)-(22b) and Eq. (32), respectively. Note that the above probability density function corresponds to a multivariate Kummer-Beta distribution whenever $\xi_k = \xi$, $1 \le k \le n_q$, in which case an explicit algebraic expression for k_0 can be obtained in terms of confluent hypergeometric functions [28]. It is worth mentioning that the result stated in Proposition 3.1 similarly holds when U follows the probability distribution defined by Eq. (33), hence ensuring the consistency of the proposed probabilistic model.

Finally, it should be pointed out that the above probability density function is a labelled but nonstandard one, for which there is no simple generator available. In this work, the adaptive algorithm proposed in [29] is used for sampling purposes.

3.4.2. Particular case of an incompressible Mooney-Rivlin material

For the incompressible Mooney-Rivlin model, the probability density function p_U of the normalized random variable U is a Kummer-Beta distribution with parameters $(\lambda_1, \lambda_2, \xi_1)$, that is:

$$p_{U}(u) = \mathbb{1}_{]0;1[}(u) \ k_0 \ u^{\lambda_1 - 1} (1 - u)^{\lambda_2 - 1} \exp\left(-\xi_1 u\right) , \qquad (34)$$

where $\lambda_1 > 1$, $\lambda_2 > 1$ and $\xi_1 \in \mathbb{R}$. It can be deduced that the normalization constant takes the form:

$$k_0^{-1} = \mathcal{B}(\lambda_1, \lambda_2) \mathcal{F}(\lambda_1, \lambda_1 + \lambda_2, -\xi_1) , \qquad (35)$$

in which \mathcal{F} stands for the confluent hypergeometric function (see e.g [25]):

$$\mathcal{F}(x, y, z) = \frac{1}{\mathcal{B}(x, y - x)} \int_0^1 u^{x-1} (1 - u)^{y - x - 1} \exp(zu) \, du , \qquad (36)$$

for all x > 0, y > 0 and $z \in \mathbb{R}$.

Upon evaluating the constraints given by Eqs. (22a), (22b) and (32) (with m = n = 1), it can be shown that the Lagrange multipliers satisfy the following set of nonlinear equations:

$$\nu_{1} = \psi(\lambda_{1}) - \psi(\lambda_{1} + \lambda_{2}) + \frac{\partial \log \left(\mathcal{F}(\lambda_{1}, \lambda_{1} + \lambda_{2}, -\xi_{1})\right)}{\partial \lambda_{1}},$$
(37a)

$$\nu_{2} = \psi(\lambda_{2}) - \psi(\lambda_{1} + \lambda_{2}) + \frac{\partial \log \left(\mathcal{F}(\lambda_{1}, \lambda_{1} + \lambda_{2}, -\xi_{1})\right)}{\partial \lambda_{2}},$$
(37b)

$$\mathbb{E}\left\{U\right\} = \frac{\lambda_1}{\lambda_1 + \lambda_2} \frac{\mathcal{F}\left(\lambda_1 + 1, \lambda_1 + \lambda_2 + 1, -\xi_1\right)}{\mathcal{F}\left(\lambda_1, \lambda_1 + \lambda_2, -\xi_1\right)} \ . \tag{37c}$$

where ψ is the Digamma function defined as [25] (see [30] for results similar to Eqs. (37a) and (37b)):

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} , \quad \forall z > 0 .$$
 (38)

In practice, solving for ξ_1 in the last equation of Eqs. (37) allows one to enforce the constraint on the mean value for given repulsion conditions (as controlled in a forward manner by λ_1 and λ_2) at the boundaries of S.

4. Numerical illustrations and model calibration with experimental data

4.1. Monte Carlo simulations without constraints on mean values

In this section, an incompressible isotropic Ogden material defined by the stochastic stored energy function given by Eq. (27) is considered. It is assumed that a coupon occupied by this material undergoes a simple tension defined by the principal stretches $v_1 = v$ and $v_2 = v_3 = v^{-1/2}$. Let Σ be the real-valued random variable corresponding to the stochastic modeling of the non-vanishing principal Cauchy stress. Upon substituting the expression of the stochastic stored energy function in the definition of the Cauchy stress, it can be shown that the random principal Cauchy stress Σ takes the form:

$$\Sigma(v) = \sum_{i=1}^{m} Q_{i} | \mathbb{L} \gamma_{i} \left(v^{\gamma_{i}} - v^{-\gamma_{i}/2} \right) + \sum_{j=1}^{n-1} Q_{m+j} | \mathbb{L} \delta_{j} \left(v^{\delta_{j}/2} - v^{-\delta_{j}} \right) + \delta_{n}^{-1} \left(2\mathbb{L} - \sum_{k=1}^{n_{q}} Q_{k} | \mathbb{L} \eta_{k}^{2} \right) \left(v^{\delta_{n}/2} - v^{-\delta_{n}} \right) .$$
(39)

for any $v \ge 0$. Below, the computation of the Lagrange multipliers for given equality constraints is not addressed: alternatively, these multipliers are considered as free model parameters and parametric studies are subsequently performed in order to illustrate the model capabilities.

4.1.1. Incompressible Neo-Hookean material

The random Cauchy stress in the case of the incompressible Neo-Hookean model is given by:

$$\Sigma(v) = \mu \left(v^2 - \frac{1}{v} \right) . \tag{40}$$

The mean value $\underline{\mu}$ of the shear modulus is chosen as $\underline{\mu} = 4.1860 \text{ kg} \times \text{cm}^{-2}$. Confidence intervals (at 90%) for the random Cauchy stress (with $v \in [1, 10]$) are shown in Fig. 1, for different values of δ_{μ} . As expected, the model allows one to generate different levels of statistical fluctuations around the given

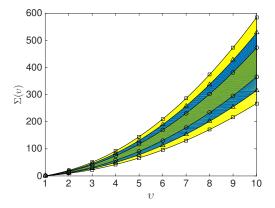


Figure 1. Confidence regions (with a probability level of 0.9) of the Cauchy stress for the incompressible Neo-Hookean model. Confidence regions are delimited by squares for $\delta_{\mu} = 0.3$, triangles for $\delta_{\mu} = 0.2$ and circles for $\delta_{\mu} = 0.1$.

mean function $v \mapsto \underline{\mu} (v^2 - 1/v)$. For a given value of δ_{μ} , the variance thus exhibited turns out to increase along with the stretch, which is in accordance with the experimental trends provided elsewhere [1] (see also the references therein).

4.1.2. Incompressible Mooney-Rivlin material

In the particular case of an incompressible Mooney-Rivlin material, the above stochastic Cauchy stress reduces to:

$$\Sigma(v) = \left(2Q|\mu + \frac{\mu - 2Q|\mu}{v}\right)\left(v^2 - \frac{1}{v}\right) , \qquad (41)$$

where $(Q|\mu=\mu):=\mu U/2$ and U follows a Beta-type I distribution with parameters $\lambda_1>1$ and $\lambda_2>1$. Confidence intervals (at 90%) for the random Cauchy stress are shown in Fig. 1 for $\lambda_1=\lambda_2=\lambda\in\{1+10^{-16},5,30\}$, $\delta_{\mu}=0.2$ (left panel) and $\delta_{\mu}=0.05$ (right panel). It is seen that due to symmetrical

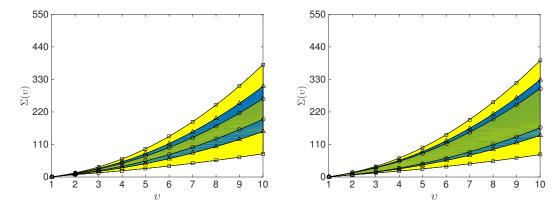


Figure 2. Confidence regions at 0.9 of the Cauchy stress for different values of $\lambda_1 = \lambda_2 = \lambda$. Square markers: $\lambda = 1 + 10^{-16}$. Triangle markers: $\lambda = 5$. Circle markers: $\lambda = 30$. Left panel: $\delta_{\mathbb{P}} = 0.05$. Right panel: $\delta_{\mathbb{P}} = 0.2$.

repulsion conditions (since $\lambda_1 = \lambda_2$), the mean function remains the same, regardless of the current value of λ (for given values of $\underline{\mu}$ and δ_{μ}). It is also found that the level of statistical fluctuations increases together with v. The evolution of the coefficient of variation for the random variable $\Sigma(10)$, denoted by $\delta_{\Sigma(10)}$ hereinafter, is shown in Fig. 3 for $\lambda_1 = \lambda_2 = \lambda \in [1 + 10^{-16}, 50]$ and $\delta_{\mu} \in \{0.05, 0.1, 0.2\}$. As

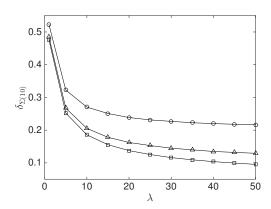


Figure 3. Graph of the coefficient of variation for the random Cauchy stress $\Sigma(10)$ w.r.t the Lagrange multipliers $\lambda_1=\lambda_2=\lambda$. Squares (\square) for $\delta_{\mathbb{p}}=5\%$, triangles (Δ) for $\delta_{\mathbb{p}}=10\%$ and circles (\circ) for $\delta_{\mathbb{p}}=20\%$.

expected, it is seen that the mapping $\lambda \mapsto \delta_{\Sigma(10)}$ is monotonically decreasing, no matter the value of $\delta_{\mathbb{P}}$, and that larger levels of fluctuations are obtained for larger values of the coefficient of variation for the

random shear modulus. Similar results are finally displayed in Figs. 5 and 4, for various combinations of λ_1 and λ_2 . It is seen for different behaviors can be emulated by properly selecting the values of the

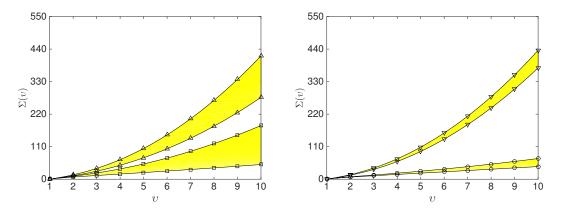


Figure 4. Confidence regions (with a probability level of 0.9) of the Cauchy stress for different sets of Lagrange multipliers (λ_1, λ_2) delimited by (left panel) (1, 5) for squares, (5, 1) for triangles, (right panel) (1, 30) for circles and (30, 1) for down triangles $(\delta_{\mu} = 0.1, \underline{\mu} = 4.1860 \text{ kg} \times \text{cm}^{-2})$.

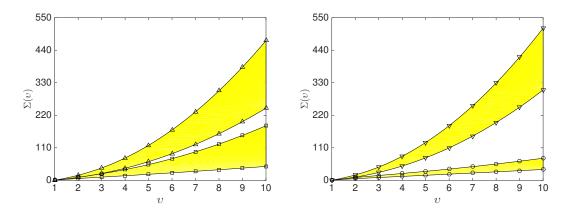


Figure 5. Confidence regions (with a probability level of 0.9) of the Cauchy stress for different sets of Lagrange multipliers (λ_1, λ_2) delimited by (left panel) (5, 1) for squares, (1, 5) for triangles, (right panel) (30, 1) for circles and (1, 30) for down triangles $(\delta_{\mu} = 0.2, \underline{\mu} = 4.1860 \text{ kg} \times \text{cm}^{-2})$.

Lagrange multipliers, hence illustrating the flexibility offered by the formulation.

4.2. Monte Carlo simulations with constraints on mean values: case of a Mooney-Rivlin material

This section is devoted to forward simulations for the stochastic representation arising from the MaxEnt formulation with repulsion and mean constraints. In the case of a Mooney-Rivlin material, the random variable U follows a Kummer-Beta distribution (defined by the probability density function given by Eq. (34)) with parameters λ_1 , λ_2 and ξ_1 (see section 3.4.2). Confidence regions of the random Cauchy stress are displayed in Fig. 6 for $\lambda_1 = \lambda_2 = 15$ and several values of ξ_1 . It is seen that whereas the additional Lagrange multiplier ξ_1 allows for specifying some mean function, its value slightly affects the

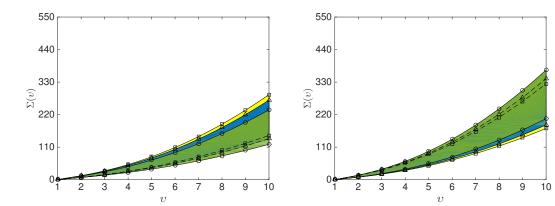


Figure 6. Confidence regions (with a probability level of 0.9) of the Cauchy stress for $\lambda_1 = \lambda_2 = 15$ and $\delta_{\mathbb{P}} = 0.2$. Left panel : $(\Box) \xi_1 = 5$, $(\Delta) \xi_1 = 10$ and $(\circ) \xi_1 = 20$. Right panel : $(\Box) \xi_1 = -5$, $(\Delta) \xi_1 = -10$ and $(\circ) \xi_1 = -20$.

level of fluctuations whenever the repulsion conditions remain fixed. In order to proceed with a target mean function while selecting a given level of fluctuations, it is then necessary to enforce that Eq. (37c) holds for arbitrary couples (λ_1, λ_2) . For illustration purposes, let us assume that the target mean value of random variable Q is given by $\mathbb{E}\{Q\} = 0.8372$, with $\underline{\mu} = 4.1860 \text{ kg} \times \text{cm}^{-2}$ and $\delta_{\mu} = 0.2$ (hence, $\mathbb{E}\{U\} = 0.4$). For any (λ_1, λ_2) in $(|1, +\infty|)^2$, ξ_1 must satisfy the equation

$$\frac{\lambda_1}{\lambda_1 + \lambda_2} \frac{\mathcal{F}(\lambda_1 + 1, \lambda_1 + \lambda_2 + 1, -\xi_1)}{\mathcal{F}(\lambda_1, \lambda_1 + \lambda_2, -\xi_1)} = 0.4 , \qquad (42)$$

which can be solved by using, for instance, a nonlinear least-square algorithm. The graph $(\lambda_1, \lambda_2) \mapsto \xi_1$ thus constructed is shown in Fig. 7. Next, confidence regions for the random Cauchy stress obtained for all these triplets are shown in Fig. 8 (left panel), where the corresponding probability density functions associated with random variable U are also shown on right panel. As expected, the probabilistic model

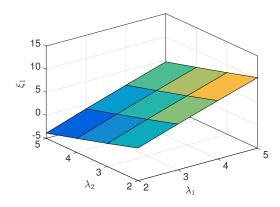
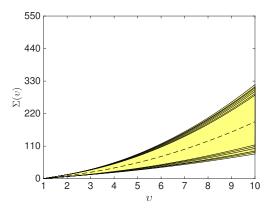


Figure 7. Graph of $(\lambda_1, \lambda_2) \mapsto \xi_1$ for all $(\lambda_1, \lambda_2) \in (\{2, 3, 4, 5\})^2$ such that $\mathbb{E}\{Q\} = 0.8372$, $\mu = 4.1860$ kg.cm⁻² and $\delta_{\mathbb{H}} = 0.2$.

allows for prescribing a desired mean function, as well as a target level of statistical fluctuations, and therefore exhibits enhanced capabilities as regards inverse identification based on (experimental) data.



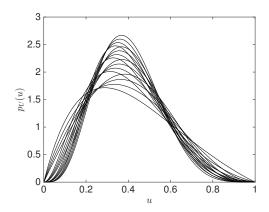


Figure 8. Confidence regions (with a probability level of 0.9) of the Cauchy stress for $(\lambda_1, \lambda_2) \in (\{2, 3, 4, 5\})^2$ (left panel). Associated probability density functions $u \mapsto p_U(u)$ (right panel).

4.3. Model calibration with experimental data

Below, we finally address the calibration of the stochastic representation defined in section 3.3, taking into account some experimental realizations. The material under consideration is a Styrene-Ethylene-co-Butylene-Styrene (SEBS) thermoplastic elastomer. Results from uniaxial quasi-static tensile tests (see [32] for details) demonstrates an isotropic and incompressible behavior, and exhibit a non-negligible variability. In practice, each realization of the stress-stretch curve is seen to be very well represented by having recourse to an Odgen-type model, with m=1 and n=2. Therefore, the stochastic stored energy function is written as

$$W([F]) = Q_1|\mathbb{\mu}\Phi_{\gamma_1}([F]) + Q_2|\mathbb{\mu}\Upsilon_{\delta_1}([F]) + \left(2\mathbb{\mu} - \gamma_1^2 Q_1|\mathbb{\mu} - \delta_1^2 Q_2|\mathbb{\mu}\right)\Upsilon_{\delta_2}([F]) , \quad \forall [F] \in \mathbb{L}_3(\mathbb{R}) , \quad (43)$$
 and depends on:

- the deterministic vector $\boldsymbol{\eta} = (\gamma_1, \delta_1, \delta_2)$ corresponding to the model exponents;
- the parameters involved in the probability distribution of the shear modulus, namely μ and δ_{μ} ;
- the Lagrange multipliers $(\lambda_1, \lambda_2, \lambda_3)$ defining the probability distribution of random variable U (see Eq. (23)).

In a first step, the mean model (as defined by η , $\underline{\mu}$ and $\underline{q} := \mathbb{E}\{Q\}$) is calibrated by imposing a nominal stress-stretch curve. The latter is obtained by fitting the mean experimental curve, making use of a classical least-square algorithm. Next, and upon using the properties of the Dirichlet-type I distribution, it can be shown that the (total) mathematical expectation of random variable Q is defined as:

$$\mathbb{E}\left\{Q_{1}\right\} = \frac{2\underline{\mu}\lambda_{1}}{\gamma_{1}^{2}\left(\lambda_{1} + \lambda_{2} + \lambda_{3}\right)} , \quad \mathbb{E}\left\{Q_{2}\right\} = \frac{2\underline{\mu}\lambda_{2}}{\delta_{1}^{2}\left(\lambda_{1} + \lambda_{2} + \lambda_{3}\right)} . \tag{44}$$

Solving for (λ_1, λ_2) in the above system then yields

$$\lambda_1 = \frac{\gamma_1^2 \underline{q}_1}{2\underline{\mu} - \gamma_1^2 \underline{q}_1 - \delta_1^2 \underline{q}_2} \lambda_3 , \quad \lambda_2 = \frac{\delta_1^2 \underline{q}_2}{2\underline{\mu} - \gamma_1^2 \underline{q}_1 - \delta_1^2 \underline{q}_2} \lambda_3 , \tag{45}$$

where only $\lambda_3 > 1$ remains unknown (and such that $\lambda_1 > 1$ and $\lambda_2 > 1$). Therefore, the Lagrange multiplier λ_3 and δ_{\parallel} can be both considered as tunable parameters, the values of which may be selected in order to enforce some level of statistical fluctuation at given stretches (in the linear part and for some large stretch, for instance). Here, and given the very limited number of realizations (which does not allow for the definition of converged statistical metrics), the values of δ_{\parallel} and λ_3 are simply calibrated so that

the experimental curves are all contained in the confidence region at 90% (see below). This confidence region, estimated for the stochastic model thus calibrated, is shown, together with the fitted experimental results, in Fig. (9).

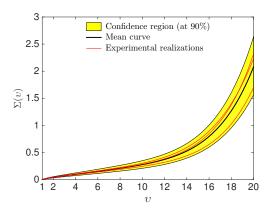


Figure 9. Confidence region (with a probability level of 0.9) of the Cauchy stress for the calibrated stochastic stored energy function.

It is seen that the stochastic representation allows for properly modeling the variability exhibited by the experimental results, for stretches up to 20.

5. Conclusion

This work has been devoted to the construction of a class of stochastic models for Odgen-type stored energy functions associated with isotropic incompressible materials. An information-theoretic methodology was proposed and involves algebraic constraints related to polyconvexity, coerciveness and consistence with linearized elasticity. Upon plugging these constraints in a maximum entropy formulation, parametric probabilistic models were defined, hence yielding stochastic stored energy functions that are covered, almost surely, by existence theorems in nonlinear elasticity. It is important to note that the methodology can be readily generalized to non-isotropic materials, provided that existence theorems hold for the case under consideration. Forwards simulations involving Neo-Hookean and Mooney-Rivlin materials were then performed and complemented with an inverse identification procedure involving experimental results. Whereas the case of random exponents could also be considered, it should be pointed out that the proposed models are shown to properly reproduce the general trends observed in experimental results, and that the case of uncertain exponents can be handled by the proposed framework (at the expense of notational complexity though). In addition, the models interestingly depend on a vector-valued hyperparameter, the low-dimension of which is intended to facilitate calibration with limited data. Finally, the generalization to compressible hyperelastic materials is worth investigating: these cases, together with procedures for statistical inverse identification, are under investigation and will be presented in a forthcoming paper.

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