

# A Bayesian Approach to Selecting Hyperelastic Constitutive Models of Soft Tissue

Sandeep Madireddy<sup>a</sup>, Bhargava Sista<sup>a</sup>, Kumar Vemaganti<sup>a,\*</sup>

<sup>a</sup>*Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio  
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## Abstract

Hyperelastic constitutive models of soft tissue mechanical behavior are extensively used in applications like computer-aided surgery, injury modeling, etc. While numerous constitutive models have been proposed in the literature, an objective method is needed to select a parsimonious model that represents the experimental data well and has good predictive capability. This is an important problem given the large variability in the data inherent to soft tissue mechanical testing.

In this work, we discuss a Bayesian approach to this problem based on Bayes factors. We propose a holistic framework for model selection, wherein we consider four different factors to reliably choose a parsimonious model from the candidate set of models. These are the qualitative fit of the model to the experimental data, evidence values, maximum likelihood values, and the landscape of the likelihood function. We consider three hyperelastic constitutive models that are widely used in soft tissue mechanics: Mooney-Rivlin, Ogden and exponential. Three sets of mechanical testing data from the literature for agarose hydrogel, bovine liver tissue, porcine brain tissue are used to calculate the model selection statistics. A nested sampling approach is used to evaluate the evidence integrals. In our results, we highlight the robustness of the proposed Bayesian approach to model selection compared to the likelihood ratio, and discuss the use of the four factors to draw a complete picture of the model selection problem.

*Keywords:* Bayesian, uncertainty quantification, soft tissue constitutive model, hyperelastic, nested sampling, Model selection

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\*Corresponding author

*Email addresses:* [madiresy@mail.uc.edu](mailto:madiresy@mail.uc.edu) (Sandeep Madireddy), [sistas@mail.uc.edu](mailto:sistas@mail.uc.edu) (Bhargava Sista), [Kumar.Vemaganti@uc.edu](mailto:Kumar.Vemaganti@uc.edu) (Kumar Vemaganti)

## 1. Introduction

### *(a). Motivation*

Hyperelastic constitutive models of soft tissue mechanical behavior find widespread use in applications like traumatic brain injury simulation, computer-aided surgery and functional tissue engineering. These models are generally phenomenological in nature and are derived from a strain energy density function that is postulated to depend on invariants of the deformation field in the elastic body. The model parameters are usually determined by a least squares fit of the constitutive model to mechanical testing data from experiments such as compression, tension [1, 2, 3], indentation [4, 5], aspiration [6, 7], etc.

For most problems, the choice of the constitutive model is driven by the quality of the fit (e.g.,  $R^2$  value) and the analyst's experience. Commonly used models include those based on strain invariants (e.g., Neo-Hookean, Mooney-Rivlin, exponential, Pucci-Saccomandi, Arruda-Boyce, etc.), or on the principal stretches (e.g., Ogden, Peng-Landel, etc.). See [8, 9] for a comprehensive list. Given this wide range of available models, an objective approach is needed to ensure that the chosen constitutive model strikes a balance between fit quality, predictive capability, and complexity. A model that is too simple may not faithfully represent the experimental mechanical response, while a model that is overly complex may be of limited use or have so many parameters that they cannot be easily identified from the available data. Thus the issue of parameter estimation is an integral part of the model selection process since the model is complete only after the parameters are estimated.

Another issue of concern in soft tissue mechanics is that the experimental data almost always have high variability, which leads to large uncertainties in the constitutive model parameters. This large variability is due to many factors: (i) soft tissue is a complex material that can be highly heterogeneous; (ii) patient to patient differences can be large; (iii) soft tissue is difficult to procure, handle and preserve, and obtaining good specimens is challenging; and (iv) experimental protocols vary widely between laboratories. These difficulties are exacerbated when the problem of interest involves irreversible and discontinuous phenomena like tissue fracture and damage, a common occurrence in injury biomechanics [10]. This variability cannot be ignored and should be systematically included in the parameter estimation and model selection process in order to obtain a reliable constitutive model.

### *(b). Model Selection Strategies*

Model selection procedures often rank the candidate models based on some widely accepted criteria. The selected model should obey the principle of parsimony or Occam's razor, which states that the simplest model that can explain the data should be accepted. That is, a balance between goodness of fit and model complexity has to be achieved. This property of the model is essential to avoid overfitting and to render the model more testable. Most model selection methods can be categorized into three groups: (a) Bayesian methods using the Bayes factor [11, 12], (b) frequentist methods that include p-value method, Mallows's

$C_p$ , etc., and (c) Information-theoretic methods like the Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and variants [13].

The Bayesian approach has some advantages over frequentist methods [14]. First, it is easier to interpret the posterior probabilities of the model and the Bayes factor as the odds of one model over the other. Second, the Bayesian approach is consistent in the sense that it guarantees the selection of the true model if it is part of the candidate model set under very mild conditions. If the true model is not present in the set, then the model closest to the true model in terms of the Kullback-Leibler divergence is chosen [15, 16].

The Bayesian approach mainly involves updating prior knowledge of the model with new experimental observations (represented by a likelihood function) to obtain the posterior distribution of the model parameters. The marginal likelihood or evidence is then obtained by marginalizing the likelihood function over the space of its existence; this is discussed in more detail in Section 3.

Bayesian model selection is a natural Occam’s razor. The use of the marginal likelihood automatically penalizes overly complex models because complex models spread their probability mass very widely and predict that everything is possible. Thus the probability of the actual data is small. This is illustrated in Fig. 1 (adapted from [17]), where the model space  $\mathfrak{M}$  consists of three models  $\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3$  with equal probabilities, each with a single parameter  $\theta$ . The data space  $\mathfrak{D}$  is assumed to be one-dimensional, and  $\mathbf{d} \in \mathfrak{D}$  is the dataset used to estimate the parameter  $\theta$ , which is assumed to be a single value. Model  $\mathbf{m}_3$  is a more complex model in the sense that it can predict more data, while model  $\mathbf{m}_1$  is the simplest. The dashed straight line corresponds to a particular observed dataset  $\mathbf{d}$ . The quantity  $P(\mathbf{d}|\mathbf{m}_i)$  represents the probability of obtaining the data given a particular model  $\mathbf{m}_i$ ; this is the marginal likelihood or evidence. The quantity  $P(\theta|\mathbf{d}, \mathbf{m}_i)$  represents the posterior probability of the parameter given the data set and model. For the example shown here, model  $\mathbf{m}_1$  is unable to predict the data, model  $\mathbf{m}_2$  predicts the data and has the highest evidence value, while model  $\mathbf{m}_3$  also predicts the data but with a lower evidence value. Thus model  $\mathbf{m}_2$  is the model of choice.

The Bayesian approach is also more general in the sense that it does not require nested models, standard distributions or any asymptotic assumptions while the other methods require at least one of these.

### (c). *Choice of the Prior*

Another important aspect of model selection and perhaps the most criticized aspect of the Bayesian framework is the specification of the prior probability distribution on the parameters. For the case of parameter estimation, the selection of the prior is not as critical when the data is informative. But in the case of model selection, the prior indeed influences the evidence integral and needs to be well justified. However this influence can be expected to decrease when the data is more informative [18].

In general, the selection of the prior is done through a sensitivity analysis based on a few appropriate priors. In the situation where the prior distribution is not exactly known, one often chooses a non-informative prior, i.e., one whose contribution to the posterior is minimal.

One approach to constructing a non-informative prior is based on the principle of indifference and the principle of insufficient reason. Here, one assumes uniform distributions on all the parameters to span an infinite range  $[-\infty, \infty]$ . This covers all possible true values of the parameters and gives them equal probability. The problem with this is that in order for the probability to sum to one, infinitely small probability has to be placed on the parameters, which when multiplied by a likelihood obtained from a low information data can lead to negligible evidence. One way to get around this is to constrain the parameter space to the bounds in which the likelihood is estimated to be appreciable. This can be done from expert opinion or by inspection in several regions of the parameter space.

Other approaches to choosing non-informative priors include:

- (a) Constructing a prior based on the invariance structure in the problem using the right Haar measure;
- (b) Constructing a prior that is invariant under reparametrization – e.g., Jeffreys prior [19];
- (c) Reference priors: Choosing a prior that maximizes the Kullback-Leibler distance between posterior and the prior [20];
- (d) Maxent priors: Choosing a prior that maximizes the entropy [21]; and
- (e) Other methods such as data-translated likelihoods, probability matching [22].

These priors generally turn out to be improper and do not integrate to one, which can be problematic [22]. One way to get around improper priors is by using partial or alternative Bayes factors [23], wherein a part of the data called the training set is used to make the prior proper. This can then be used as an informative prior for the rest of the data. Some of the ways to obtain partial Bayes factors include pseudo-Bayes factor [24], posterior Bayes factor [25], intrinsic Bayes factor [26], and fractional Bayes factor [27].

*(d). Evidence Integral Evaluation*

Although Bayesian model selection has many advantages over other approaches, one of its major drawbacks is the cost of evaluating the multidimensional evidence integral. The evidence integral can be evaluated analytically only for a few cases in which the closed form of the posterior is available. For example, this is possible for the exponential family distributions with conjugate priors [11]. Under the assumption of large data, asymptotic approximation methods (Laplace method, Schwarz method) can be used.

In the case of more complicated distributions, sampling-based methods like simple Monte Carlo, importance sampling, Markov Chain Monte Carlo (MCMC) and its variants like delayed rejection adaptive metropolis (DRAM) [28], or differential evolution adaptive metropolis (DREAM) [29] can be used. These methods are computationally expensive, and tend to

have problems with sampling efficiency for high dimensional multimodal distributions with large degeneracies between parameters. Also the proposal distribution needs to be carefully tuned for efficiency, and checking for convergence can be problematic [30]. Adaptive quadrature-based methods [31] are suitable for low dimensions. Some fast approximating methods include thermodynamic integration, Gaussian approximation of each mode, Savage-Dickey ratio, and bridge sampling, but they are only suitable for a few special situations [32]. One of the more recent and efficient sampling-based methods is the nested sampling approach [33]. This along with its implementation MULTINEST [30] has been shown to be more efficient than the aforementioned methods, and can be used to obtain the evidence value and the parameter estimates simultaneously. This is the approach employed in our study.

*(e). Bayesian Model Selection for Phenomenological Models*

The Bayesian model selection procedure has not been explored in depth in the context of soft tissue constitutive models. For phenomenological models in general, Prudencio et al. [34] used this approach to select between two competing continuum damage models to predict the failure in a composite material wherein a parallel adaptive multilevel sampling algorithm [35] is used to calculate the evidence integral. Oden et al. [36] used a similar procedure to select between two phenomenological models of tumor growth in living tissues using synthetic data. For structural dynamics problems, Beck and Yuen [37], Beck [38], and Yuen [39] advocated the use of asymptotic approximations of the evidence integral to calculate Bayes factors for globally identifiable cases (large data sets) and MCMC-based methods for globally unidentifiable cases (small data sets).

Elsheikh et al. [40] used a nested sampling-based Bayesian model selection approach to choose the number of terms in the Karhunen-Loève (KL) expansion to build a surrogate for subsurface flow models. Hadjidoukas et al. [41] used the transitional MCMC (TMCMC) method to calculate the evidence integral to select among three discrete element method models used to simulate a granular material. Sandhu et al. [42] calculated the evidence integral for 60 different nested models that describe the response of nonlinear aeroelastic oscillatory systems. Chib-Jeliazkov estimator [43] calculated using parallel adaptive MH based MCMC algorithm is used to evaluate the evidence integral.

Evidence integral calculation based on MULTINEST algorithm is more widely used in the field of cosmology [18]. Martin et al. [44] used this procedure to choose between two different classes of models that describe the cosmological inflationary potential. Feroz et al. [32] used it to select among two variants of constrained minimal supersymmetric standard model. In the field of systems biology, Pullen and Morris [45] used nested sampling based on MULTINEST for model selection among four different models.

*(f). Current Research*

In this article, we address the question of model selection and ranking among competing soft tissue constitutive models based on the Bayesian framework. Specifically, three phe-

nomenological constitutive models (Ogden, Mooney-Rivlin and exponential) that describe the hyperelastic response of soft tissue are considered. For the multi-term Ogden model, we consider  $N = 1, 2, 3$ . This allows us to perform two types of comparisons among the models: models of the same form but different levels of complexity, and models of the same complexity but different forms. Three sets of mechanical testing data from the literature are used: agarose hydrogel, bovine liver tissue, porcine brain tissue. For each dataset, we calculate the model parameters for each of the aforementioned phenomenological models using Bayesian inference, and evaluate evidence values and Bayes factors. We then rank the models using two scales: Bayes factors and likelihood ratios. We use the nested sampling algorithm MULTINEST [30] to evaluate the evidence integrals. Two distinct priors are considered: uniform prior and Gaussian prior. This allows us to study the effect of the prior on the model selection statistics and determine Bayesian robustness.

We propose a holistic approach for model selection, wherein we consider four important factors to reliably choose a parsimonious model from the candidate set of models. These are: the fit of the model with the maximum likelihood parameters to the data, evidence values, maximum likelihood values, and the landscape of the log-likelihood function. Each of these factors provides a different piece of information about the model. A good fit ensures that the model is adequate to capture the physics of the problem, while the log-likelihood value quantifies the goodness of the fit. A high evidence value provides a balance between goodness-of fit and model complexity, while the landscape of the likelihood function provides clues to any overfitting issues. These four pieces of information have to be considered together in order to find a parsimonious model in the candidate set (provided such a model exists among the candidates).

We compare the model rankings that results from the two model selection criteria for each of the datasets. Our results show that a model selection approach based on the Bayes factor is a robust way to carry out model selection when the evidence integral evaluation and the sensitivity to the prior probability are properly addressed.

The paper is structured as follows. Following this Introduction, Section 2 describes the characterization of the material behavior of soft tissues and the constitutive models used in this study. In Section 3 we introduce the Bayesian model selection framework and its different components adopted in this work. In Section 4, we present the experimental data and the model selection statistics obtained for various constitutive models and datasets. This is followed by a discussion of the results in Section 5 and some concluding remarks in Section 6.

## 2. Materials and Methods

In this study, the deformation of soft tissue is modeled using the continuum mechanics framework. We assume that soft tissue is an isotropic incompressible hyperelastic medium.

Though soft tissue is often viscoelastic and anisotropic [46, 47], we make the assumption of hyperelasticity to simplify the analysis.

(a). *Continuum Mechanics*

Let  $\mathbf{X}$  and  $\mathbf{x}$  be the reference and current coordinates of a particle in the body undergoing deformation  $\mathbf{x} = \chi(\mathbf{X})$ . The deformation gradient defined as  $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ , and the right Cauchy-Green deformation tensor is  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ . The eigenvalues of  $\mathbf{F}$  are the principal stretches and denoted  $\lambda_k$ ,  $k = 1, 2, 3$ . Then the eigenvalues of  $\mathbf{C}$  are given by  $\lambda_k^2$ . The principal invariants of  $\mathbf{C}$  are

$$I_1(\mathbf{C}) = \text{trace}(\mathbf{C}), \quad I_2(\mathbf{C}) = \frac{1}{2}((I_1(\mathbf{C}))^2 - \text{trace}(\mathbf{C}^2)), \quad I_3(\mathbf{C}) = \det(\mathbf{C}). \quad (1)$$

For a hyperelastic material, the strain energy density function  $\Psi$  can be expressed in terms of the right Cauchy-Green deformation tensor  $\mathbf{C}$ , or principal stretches  $\lambda_i$

$$\Psi = \Psi(\mathbf{C}) = \Psi(\lambda_1, \lambda_2, \lambda_3) \quad (2)$$

For an incompressible isotropic material, the second Piola-Kirchhoff stress tensor  $\mathbf{S}$  can be obtained from  $\Psi$  using the expression

$$\mathbf{S} = -p\mathbf{C}^{-1} + 2\frac{\partial \Psi}{\partial \mathbf{C}} \quad (3)$$

where  $p$  is a Lagrange multiplier term. Subsequently the Cauchy stress tensor can be obtained from  $\mathbf{S}$  as

$$\boldsymbol{\sigma} = \mathbf{F}\mathbf{S}\mathbf{F}^T = -p\mathbf{I} + 2\mathbf{F}\frac{\partial \Psi}{\partial \mathbf{C}}\mathbf{F}^T \quad (4)$$

In this study, the hyperelastic response is characterized using three different phenomenological constitutive models. They are the Mooney-Rivlin model, the Ogden model, and the exponential model.

The strain energy density function and the corresponding uniaxial stress for the Mooney-Rivlin model  $\Psi$  are given by

$$\Psi = C_1(I_1 - 3) + C_2(I_2 - 3) \quad (5)$$

$$\sigma_{11}(\lambda) = \left(2C_1 + \frac{2C_2}{\lambda}\right) \left(\lambda - \frac{1}{\lambda^2}\right) \quad (6)$$

where  $I_1$  and  $I_2$  are the first and the second principal invariants of  $\mathbf{C}$ ,  $\lambda$  is the stretch in the direction of loading, and  $C_1$  and  $C_2$  are the model parameters. The shear modulus of the material is  $\mu = 2(C_1 + C_2)$ .

For the Ogden model, the strain energy density function and the uniaxial stress are given by

$$\Psi = \sum_{i=1}^N \frac{2\mu_i}{\alpha_i^2} (\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3) \quad (7)$$

$$\sigma_{11}(\lambda) = \sum_{i=1}^N \frac{2\mu_i}{\alpha_i} (\lambda^{\alpha_i-1} - \lambda^{-\frac{\alpha_i}{2}-1}) \quad (8)$$

where  $\mu_i$  and  $\alpha_i$  are model parameters and the value of  $N$  specifies the order of the model. The shear modulus of the material is given by  $\mu = \sum_{i=1}^N \mu_i$ .

Finally, for the exponential model, the strain energy density function and the resulting uniaxial stress are given by

$$\Psi = B_1(\exp(B_2(I_1 - 3)) - 1) \quad (9)$$

where  $B_1$  and  $B_2$  are now the model parameters. The uniaxial Cauchy stress is

$$\sigma_{11}(\lambda) = 2 \left( \lambda - \frac{1}{\lambda^2} \right) B_1 B_2 \exp \left( B_2 \left( \lambda^2 + \frac{2}{\lambda} - 3 \right) \right) \quad (10)$$

where  $B_1$  and  $B_2$  are the model parameters and the shear modulus is proportional to the product of the parameters:  $\mu = K B_1 B_2$ .

The Mooney-Rivlin model, the exponential model and the Ogden model with  $N = 1$  have the same complexity in the sense that they are all characterized by two material parameters. On the other hand, the Ogden model with  $N = 1$ ,  $N = 2$  and  $N = 3$  leads to models of different complexities characterized by two, four, and six parameters, respectively.

### 3. Model Selection

#### (a). Model Selection Framework

Assume  $\mathfrak{G}$  to be the physical system under study, and model space  $\mathfrak{M}$  represent the space of all models that characterize the system. Every model  $\mathbf{m}_k$  from the space  $\mathfrak{M}$  is a functional form  $f(\boldsymbol{\theta}|\mathbf{m}_k)$  with a fixed number of parameters  $\boldsymbol{\theta}$ . Let  $\mathfrak{D}$  be the data space which is the space of all possible instrument responses.

We hypothesize that the model and the data are related through

$$f(\boldsymbol{\theta}|\mathbf{m}_k) = \mathbf{d} + \boldsymbol{\eta} \quad (11)$$

where  $\mathbf{d} \in \mathfrak{D}$  is the hypothetical true data, and  $\boldsymbol{\eta}$  is the noise that contributes uncertainty to any experiment or observation that involves measurements. For soft tissue, this noise generally arises from a combination of the inherent variability in the material, its environment, and the measurement itself. Note that  $\mathbf{d} + \boldsymbol{\eta}$  is the actual system response obtained

from the experiment. We assume for simplicity that the data  $\mathbf{d}$  is known in the form of a mean vector  $\mathbf{D}$  and a vector of standard deviations  $\mathbf{\Delta}$ . Let the cardinality of the candidate set of models be  $N$ , the prior probability of each model to be  $P(\mathbf{m}_k|I)$ . Assuming that  $\sum_{k=1}^N P(\mathbf{m}_k|I) = 1$ , from Bayes theorem it follows that

$$P(\mathbf{m}_k|\mathbf{d}, I) = \frac{P(\mathbf{d}|\mathbf{m}_k, I)P(\mathbf{m}_k|I)}{\sum_{k=1}^N P(\mathbf{d}|\mathbf{m}_k, I)P(\mathbf{m}_k|I)} \quad (12)$$

To ascertain the relative merits of a pair of models  $\mathbf{m}_k, \mathbf{m}_j$  the ratio of their posteriors in light of the experimental data is calculated as

$$\frac{P(\mathbf{m}_k|\mathbf{d}, I)}{P(\mathbf{m}_j|\mathbf{d}, I)} = \frac{P(\mathbf{d}|\mathbf{m}_k, I) P(\mathbf{m}_k|I)}{P(\mathbf{d}|\mathbf{m}_j, I) P(\mathbf{m}_j|I)} \quad (13)$$

or

$$\text{Posterior odds} = BF_{kj} \times \text{Prior odds} \quad (14)$$

where  $BF_{kj}$  is the Bayes factor, which transforms the prior odds into the posterior odds in light of the data  $\mathbf{d}$ . Here,  $P(\mathbf{d}|\mathbf{m}_k, I)$  is called the marginal likelihood or evidence, and is obtained by marginalizing the posterior of the parameters for a given model  $P(\boldsymbol{\theta}_k|\mathbf{d}, m_k, I)$  over its parameter space  $\boldsymbol{\theta}_k$ .

$$P(\mathbf{d}|m_k, I) = \int_{\boldsymbol{\theta}_k} P(\mathbf{d}|\boldsymbol{\theta}_k, m_k, I)P(\boldsymbol{\theta}_k|m_k, I) d\boldsymbol{\theta}_k \quad (15)$$

The quantity  $P(\mathbf{d}|\boldsymbol{\theta}_k, m_k, I)$  is called the likelihood function, which gives the likelihood of observing the data  $\mathbf{d}$  given the parameters  $\boldsymbol{\theta}_k$ , and  $P(\boldsymbol{\theta}_k|m_k, I)$  is the prior knowledge about the parameters before the experimental data are obtained.

The evidence can be seen as the probability mass (volume) contained under the posterior probability distribution over the parameter space for a given model. The value of the evidence would be higher for a model if more of its parameter space is at a higher likelihood than the model for which the likelihood distribution is highly peaked for a small parameter space and the rest of it has a low likelihood values.

*(b). Choice of the Likelihood Function*

The data in this study is obtained from experimental measurements on soft tissue and hydrogels. The noise associated with the experimental measurements,  $\boldsymbol{\eta}$ , can reasonably be represented as a Gaussian process based on maximum entropy considerations [48]. The likelihood function, which is a joint distribution of this experimental data assuming the data are independent and identically distributed (i.i.d) can be written as

$$P(\mathbf{d}|\boldsymbol{\theta}_k, m_k, I) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\Delta_i^2}} \exp \left[ -\frac{(f(\boldsymbol{\theta}_k|\mathbf{m}_k) - D_i)^2}{2\Delta_i^2} \right] \quad (16)$$

where  $n$  is the number of points at which the data are measured. It is better to work with the logarithm of the likelihood than with the likelihood function itself since it varies slowly with respect to the parameters. The logarithm of the likelihood is given by

$$\log [P(\mathbf{d}|\boldsymbol{\theta}_k, m_k, I)] = \sum_{i=1}^n -\frac{1}{2} \log(2\pi\Delta_i^2) - \sum_{i=1}^n \left[ \frac{(f(\boldsymbol{\theta}_k|\mathbf{m}_k) - D_i)^2}{2\Delta_i^2} \right] \quad (17)$$

(c). *Algorithm to Evaluate the Evidence Integral*

As mentioned earlier, we use Nested Monte Carlo sampling based algorithm, MULTINEST to evaluate the evidence integral. It is a Monte Carlo technique used to estimate Bayesian evidence, wherein the parameter estimates are obtained as a by-product. The evidence is calculated by transforming the multi-dimensional evidence integral over the parameter space into a one-dimensional integral over the likelihood space. This is illustrated in Fig. 2.

Adopting the terminology of [30], a differential element of the prior “mass“ is defined by  $dX = \pi(\Theta)d\Theta$ , where  $\pi(\Theta)$  is the assumed prior distribution. The prior volume is obtained from the expression

$$X(\lambda) = \int_{\{\theta:\mathcal{L}(\theta)>\lambda\}} \pi(\Theta)d\Theta \quad (18)$$

which is the proportion of the prior with likelihood greater than  $\lambda$ . Subsequently, the evidence integral can be calculated using the prior volume to be

$$\mathcal{Z} = \int_0^\infty X(\lambda)d\lambda$$

When  $\mathcal{L}(X)$ , the inverse of  $X(\lambda)$  exists, i.e.,  $\mathcal{L}(X(\lambda)) = \lambda$ , the evidence can be rewritten as

$$\mathcal{Z} = \int_0^1 \mathcal{L}(X)dX$$

This is the area under the  $X - \mathcal{L}$  curve, as seen in Fig 2.

The overall algorithm can be written as [30]:

1. Sample the prior on parameters  $n$  times to get a set of  $n$  sample points (active points)
2. Calculate likelihood for each point
3. Sort the points based on the likelihood
4. Calculate the evidence for the set
5. Remove the point with the lowest likelihood ( $\mathcal{L}^*$ )
6. Generate a new sample point from the prior subjected to the constraint  $\mathcal{L}(\Theta) > \mathcal{L}^*$
7. Calculate the evidence for the new set

8. Check if the difference between the current and the previous evidence is within a tolerance
9. If yes, exit. Else go to step 3

Generating unbiased samples efficiently from the prior subject to the constraint in step 6 is a major challenge in the nested sampling algorithm. MULTINEST uses the simultaneous ellipsoidal rejection sampling scheme to address this challenge. In this sampling scheme, the set of active points at every iteration are partitioned into clusters, and ellipsoids are constructed around them using the expectation-minimization (EM) algorithm discussed in [30] to approximate each cluster. A new sample is generated from the union of these ellipsoids such that it satisfies the constraint in step 6. This algorithm reliably isolates the multiple modes and evaluates the statistics for each mode separately. We set the number of live points to 4000 and the convergence tolerance as 0.01 [32].

*(d). Choice of Prior Probability Distribution Function*

In this study, we use two different priors: the uniform prior  $\mathcal{U}(-100, 100)$  and the Gaussian prior  $\mathcal{N}(0, 100)$  over all the parameters to study the sensitivity of the maximum likelihood and evidence to the prior choice. The range of the uniform prior is carefully chosen to be large enough to encompass the parameter space in which the likelihood is appreciable. Also it should be noted that nested sampling algorithm generate samples from the parameter space of the prior, so improper priors over long ranges cannot be handled efficiently.

*(e). Interpretation of the Bayes Factor*

The Bayes factor represents the evidence provided by the data in favor of one hypothesis or model over the other. The values of the Bayes factors can be interpreted based on Jeffreys scale, which is shown in Table 1 [11].

## 4. Results

*(a). Experimental Data*

The three different data sets used in this study are obtained from the literature. These data sets correspond to agarose hydrogel [49], bovine liver tissue [50], and porcine brain tissue [51]. The details of the experimental testing is summarized in Table 2. For each dataset, we obtain parameter estimates for the three hyperelastic material models and study the model selection aspects discussed earlier. Note that all three sets of data involve low strain rates, which allows us to ignore any viscoelastic effects and idealize the materials as hyperelastic.

(b). *Model Fits*

The maximum likelihood estimate (MLE) is obtained for each of the candidate models (Mooney-Rivlin, exponential and Ogden ( $N = 1, 2, 3$ )) for the three sets of experimental data using MULTINEST. The resulting fits to data A using these MLE are shown in Fig. 4. Qualitatively, the fits for Mooney-Rivlin, exponential, and Ogden ( $N = 1$ ) models are poor, whereas the Ogden ( $N = 2, 3$ ) models provide good fits.

Similarly the model fits for Data B are shown in Fig 5. The Mooney-Rivlin model provides a poor fit, whereas the exponential and Ogden ( $N = 1, 2, 3$ ) models result in good fits.

The results for for Data C are shown in Fig. 6. Mooney-Rivlin, Ogden ( $N = 1$ ), and exponential models lead to poor fits. Ogden ( $N = 2, 3$ ) models provide qualitatively good fits.

(c). *Log-Likelihood Function, Log-Evidence, and Bayes Factors*

The values of the log-likelihood function corresponding to the MLEs for each of the models for the three data sets are shown in Table. 3. For each case, these values are obtained using two priors: uniform prior and Gaussian prior. There is no discernible difference in the values obtained from the two priors. For Data A, the Mooney-Rivlin, exponential and Ogden ( $N = 1$ ) models all show very low log-likelihood values, which is not surprising given the poor fits obtained from these models. A similar situation exists with Data B, where good visual fits correspond with high log-likelihood values.

For Data C, however, the situation is different. All models have comparable log-likelihood values even though the fits from Ogden ( $N = 2, 3$ ) seem clearly better (qualitatively speaking) than the rest.

In Table 4, we list the values of the evidence integral for all the cases. The evidence integral is calculated using MULTINEST , with the tolerance value for log-evidence set at 0.01. Additionally, the software estimates the error in the integral, which is also shown in the table.

Bayes factors are calculated for all the models with respect to the model that has the highest value of evidence. For data A, the model with the highest evidence value is the Ogden ( $N = 2$ ) model, while the Ogden ( $N = 1$ ) model has the highest evidence for Data B and Data C. The resulting values of the Bayes factors are classified based on the Jeffreys scale, which is shown in Table 5.

Next, we rank the candidate models based on the Bayes factors and the classical log-likelihood ratios. The ranks for Data A, Data B, and Data C are shown in Tables 6, 7, and 8, respectively. In all cases, the two criteria lead to different rankings of the models. In particular, for Data C, the difference is dramatic and the rankings of the models by the two criteria are completely reversed. The model considered the best by the Bayes factor criterion is the worst one according to the log-likelihood ratio and vice versa.

Additionally we look at the landscape of the likelihood function (based on the work by [52]) as a crucial criterion to consider in the model selection process. For Data A, The log-likelihood function shows distinct peaks for the Mooney-Rivlin, exponential, and Ogden ( $N = 1, 2$ ), but shows a relatively flat likelihood surface for Ogden ( $N = 3$ ). For Data B, distinct peaks are obtained for Mooney-Rivlin, exponential, and Ogden ( $N = 1$ ) but the log-likelihood surface is flat for Ogden ( $N = 2, 3$ ). The landscape of the log-likelihood functions for the five models for Data C is similar to that of Data B.

## 5. Discussion

### (a). *Dependence on the Prior*

For the data and models considered here, the maximum value (peak) of the log-likelihood function is insensitive to the change in the prior (Table 3), and so are the corresponding values of the MLE. This means the data is informative enough that the obtained values of the MLE are data driven rather than prior driven. Thus one can have more confidence in the values of MLE and the maximum log-likelihood.

The values of the marginal likelihood (evidence) for the various models do not change significantly with the prior, as seen from Table 4. For a given dataset, the small differences in the evidence values from the two priors do not change the evidence ratios and thus the Bayes factors (Table 5) and ranks remain unchanged.

### (b). *Model Selection: Four Factors*

There are four factors that should be considered in the Bayesian framework for model selection to find a parsimonious model that balances model complexity and goodness of fit:

1. The qualitative fit of the model (with the MLE parameters) to the data. The fit “quality” is generally subject to the analyst’s judgement.
2. The maximum log-likelihood values. This is a quantitative measure of the goodness of fit. This is not an absolute measure but can be used to compare models.
3. The log-evidence values. This quantifies the likelihood of the data given the model, and a higher value of evidence means that the data are more likely to be predicted by the model. The ratio of evidences is the Bayes factor.
4. The landscape of the log-likelihood function. A flat log-likelihood function is undesirable because the model parameters are more difficult to identify uniquely.

Ideally, a parsimonious model should have a good fit to data, high values of log-likelihood and log-evidence, and a log-likelihood function that is not flat. For some problems, it may not be possible to satisfy all of these requirements. In such cases, the Bayes factor can be used as a rational basis for making model selection decisions. We discuss these issues next.

The models used in this study can be grouped into two classes:

1. Models with the same functional form but increasing complexity with increasing number of terms. This is the case with the Ogden ( $N = 1, 2, 3$ ) models, where a model of order  $N$  has  $2N$  parameters.
2. Models with same complexity but different functional forms. For this we consider Mooney-Rivlin, exponential, and Ogden ( $N = 1$ ), all of which have two parameters.

*(b).1. Models with Increasing Complexity*

For the cases considered here and in general, the maximum log-likelihood value increases with an increase in the complexity of the model. This can be seen for all the three datasets for Ogden ( $N = 1, 2, 3$ ) in Table 3. But the log-likelihood does not address the question of “overfitting,” i.e., is the model more complex (and thus has more parameters) than necessary. Addressing this issue is essential to selecting a parsimonious model. One way to avoid overfitting is through the use of terms that penalize overly complex models. Current approaches in the literature that use this technique assume large data sets and asymptotics [13], and are of limited use for the problem at hand. In contrast to the log-likelihood, the marginal likelihood or evidence is a natural Occam’s razor as discussed in the Introduction. Put another way, the evidence value increases till sufficient complexity is reached and decreases beyond that.

For Data B, Ogden ( $N = 1, 2, 3$ ) all provide good fits. However, the evidence value decreases from Ogden ( $N = 1$ ) to Ogden ( $N = 2$ ), and decreases further for Ogden ( $N = 3$ ). Meanwhile the corresponding log-likelihood values increase with  $N$ . This indicates that Ogden ( $N = 1$ ) satisfies the principle of parsimony for Data B, and the other two lead to overfitting. This behavior is clearly seen in the landscape of the log-likelihood functions for these models. In Fig. 7, the likelihood plots for Ogden ( $N = 1$ ) parameters have distinct peaks, whereas the model parameters for Ogden ( $N = 2, 3$ ) (seen in Figs. 8 and 9) have flat likelihoods. This means these models overfit the data, which makes parameter identification difficult, especially when a local optimization method is used to estimate them (rather than the global MULTINEST approach employed here).

For Data A, the Ogden ( $N = 1$ ) model performs poorly, while Ogden ( $N = 2, 3$ ) both provide good fits (see Fig. 4). The evidence value increases from Ogden ( $N = 1$ ) to Ogden ( $N = 2$ ) and then decreases for Ogden ( $N = 3$ ), indicating that the latter overfits the data. As with Data B discussed above, the likelihood plots confirm the overfitting. These are however not shown here for the sake of brevity, but may be found in [52].

For Data C, Ogden ( $N = 1$ ) does not provide a good fit, but Ogden ( $N = 2, 3$ ) do. However, the evidence value for Ogden ( $N = 1$ ) is higher than Ogden ( $N = 2, 3$ ), which means that the latter models overfit the data. (This is confirmed by the flat log-likelihood plots for Ogden ( $N = 2, 3$ ) in [52]). Thus, there is no parsimonious model among the candidates; they either under-fit the data (as seen from the model fit in Fig. 5) or overfit the data as indicated by the decreasing evidence values and flat log-likelihoods. Indeed, for this particular dataset with the given levels of noise, the ideal model would lie (in complexity)

between Ogden  $N = 1$  and Ogden  $N = 2$ .

To illustrate the role of the noise on model selection and ranking, we consider the same dataset but with one-sixth the original experimental variance. The resulting values of maximum log-likelihood and evidence are shown in Table 9. This time, Ogden ( $N = 2$ ) has all four properties described earlier, and emerges as the best among the candidates. The corresponding fits to the experimental data are shown in Fig. 10. The exponential, Mooney-Rivlin and Ogden ( $N = 1$ ) models all have poor fits and low evidence values, while the more complex Ogden ( $N = 3$ ) provides a good fit but shows a lower evidence value than the Ogden ( $N = 2$ ).

### *(b).2. Models with the Same Complexity*

For Data A, none of the candidate models (Mooney-Rivlin, exponential, and Ogden ( $N = 1$ )) provide a good fit to the data. This results in very low log-likelihood and evidence values – see Tables 3 and 4.

For Data B, the Mooney-Rivlin model provides a poor fit to the data with a low value of log-likelihood and is not considered further. For the other two models, the parameter distributions are shown in Figs. 7 and 11. Comparing these two, the exponential model has a higher log-likelihood value, while the Ogden ( $N = 1$ ) model has a higher value of evidence. This is because the likelihood function for the exponential model is highly peaked near a small area around the MLE in the parameter space, but has low values in the rest of the parameter space. Therefore, its marginal likelihood, which is the integral of the probability mass in parameter space, is small. On the other hand, for Ogden ( $N = 1$ ), the region of the log-likelihood function with appreciable log-likelihood values is larger, and leads to a higher marginal likelihood value. This shows that maximum likelihood ratio is by itself not an objective criterion for ranking or selecting models, even when the models are of the same complexity.

For data C, Mooney-Rivlin, exponential, and Ogden ( $N = 1$ ) models all under-fit the data. Their maximum log-likelihoods are lower than the higher complexity models, but the evidence values are higher. This means the Bayesian approach based on evidence prefers lower complexity models over higher complexity models in the absence of an optimal parsimonious model.

### *(c). Model Ranking*

As we move from class 1 to class 4 based on the Jeffreys scale, the investigator has more confidence in the chosen model over the alternatives. In this study, for Data A, Ogden ( $N = 2$ ) is the best among the candidates with the odds of  $\exp(4.580) = 97.5144$  compared to the next best model. It satisfies all the criteria described earlier: good fit, high likelihood and evidence values, and a non-flat likelihood landscape. This gives us high confidence in this model.

For Data B, the Ogden ( $N = 1$ ) has an odds of  $\exp(2.2530) = 9.5162$  over the exponential model. It too satisfies the criteria laid out earlier and is thus ranked the best among the candidate models.

However for Data C, the situation is more complex mainly because of the large amount of noise in the experimental data. The Ogden ( $N = 1$ ) and exponential models under-fit the data, but their fits still lie within the error bars in Fig. 3. The Ogden ( $N = 2, 3$ ) models represent the trend in the data more faithfully and capture the curvature accurately. However, they over-fit the data and have low evidence values, and are therefore ranked lower on the Jeffreys scale. For this data set, none of the candidate models satisfies all the criteria laid out earlier.

## 6. Conclusions

In this work, we study the Bayesian approach to model selection and ranking among a set of five different models for the hyperelastic response of soft tissues. These include models of varying complexities: the Mooney-Rivlin model, the exponential model, and the Ogden model ( $N = 1, 2, 3$ ). Three different sets of mechanical testing data are considered that describe the uniaxial deformation of agarose gel, bovine liver tissue, and porcine brain tissue.

Model selection and parameter estimation should not be considered as a separate steps but should be considered as a single framework used to find a reliable model that can be used to predict the quantities of interest (QOI). We advocate the Bayesian approach to model selection using the Bayes factors because of its numerous advantages over the traditional methods along with its inherent capacity to handle the experimental noise. In the Bayesian framework we advocate the use of nested sampling based algorithm MULTINEST for its inherent global optimization and efficient evidence evaluation (for a detailed discussion on the global optimization of MULTINEST in the context of parameter estimation, refer to [52]).

Another important aspect is the sensitivity of the likelihood function to the choice of the prior (Bayesian robustness) to ascertain that posterior distribution is data dominated rather than prior dominated. In our study, we used two priors namely, uniform prior and gaussian prior and found that the values of maximum log-likelihood, MLE and log-evidence are insensitive to the prior increasing the confidence in our results.

In this study, four important factors are considered simultaneously to reliably choose a parsimonious model from the candidate set of models. These are the fit of the model (with the MLE parameters) to the data, log-evidence values, maximum log-likelihood values, and the landscape of the log-likelihood function. While the importance of the model fit is obvious, log-evidence values help pick a parsimonious model that balances goodness of fit and model complexity, while further insight into the overfitting of a model is obtained by looking at the landscape of the log-likelihood function. This is flat when the model overfits the data and

peaked when not. Also maximum log-likelihood values give information about the goodness of fit. This information can be effectively used to determine whether a parsimonious model is present in the candidate model set (as in the case of Data A and Data B), or if none of the models in the set are parsimonious (as in the case of Data C).

Our results show that the Bayes factor is a more reliable criterion than the likelihood ratio for choosing between models and is a robust method to do model selection when the evidence integral evaluation and the sensitivity to the prior probability are properly addressed. The Bayes factors can be used to conveniently rank the models in the order of usability to provide further insight to the investigator. This method is general and can be used for any combination of data and constitutive model.

## 7. Acknowledgements

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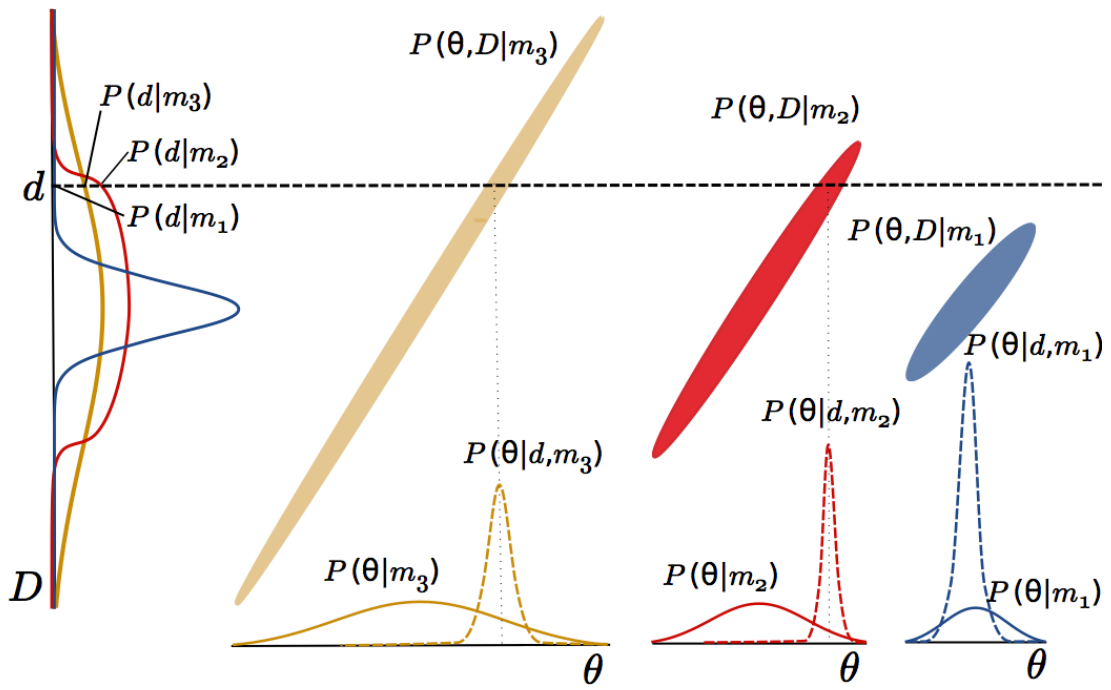
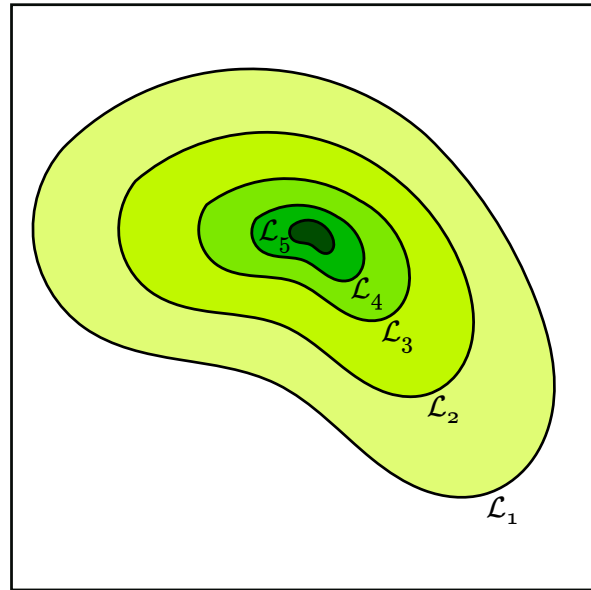
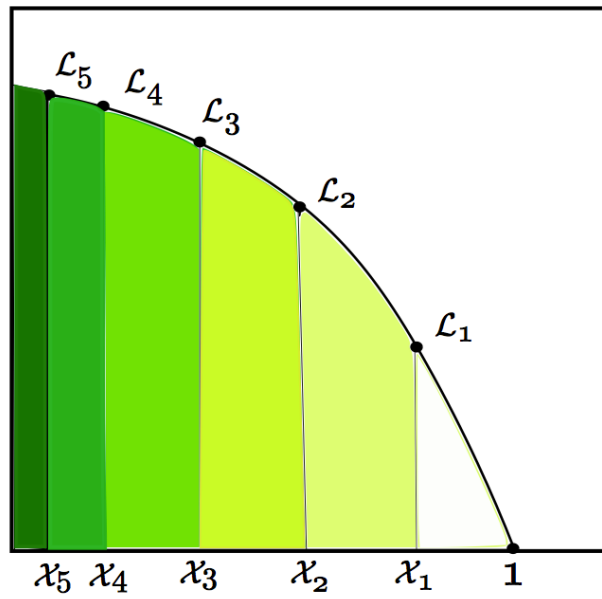


Figure 1: Occam's Razor: Figure adapted from [17].

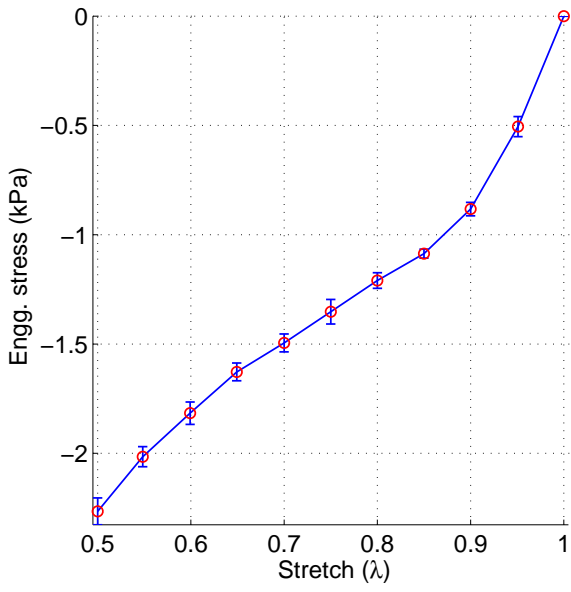


(a)

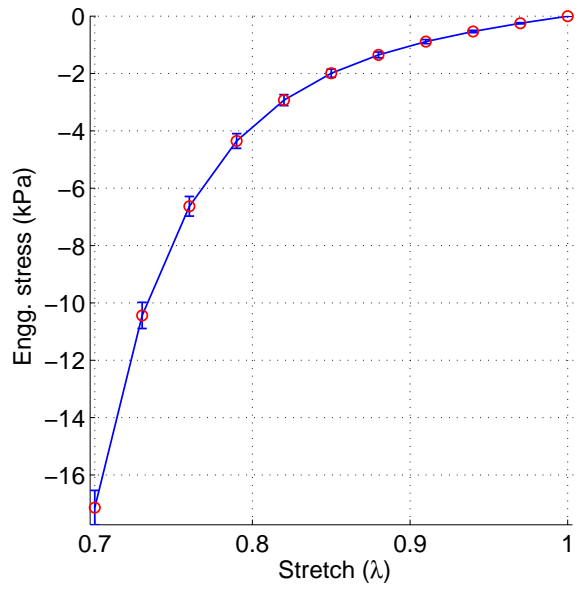


(b)

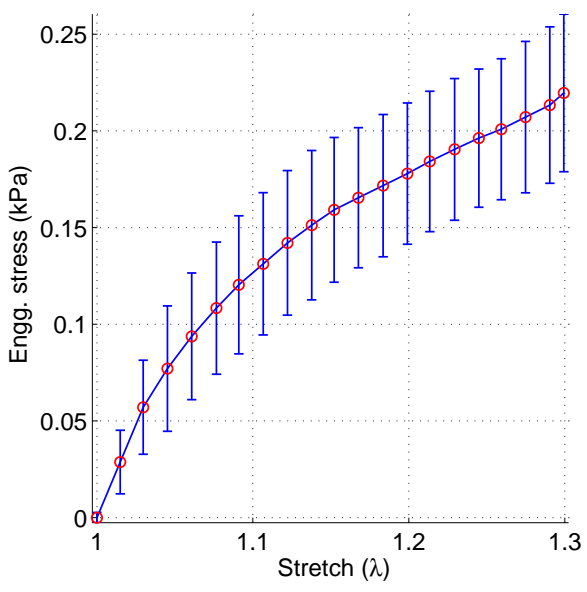
Figure 2: Schematic of the nested sampling approach: (a) Contours of likelihood function, and (b) Likelihood as a function of the prior volume  $X$ .



(a)



(b)



(c)

Figure 3: Experimental stress-strain data used in the study: (a) Data A: Unconfined compression of agarose, (b) Data B: Uniaxial compression of bovine liver, and (c) Data C: Uniaxial extension of porcine brain tissue

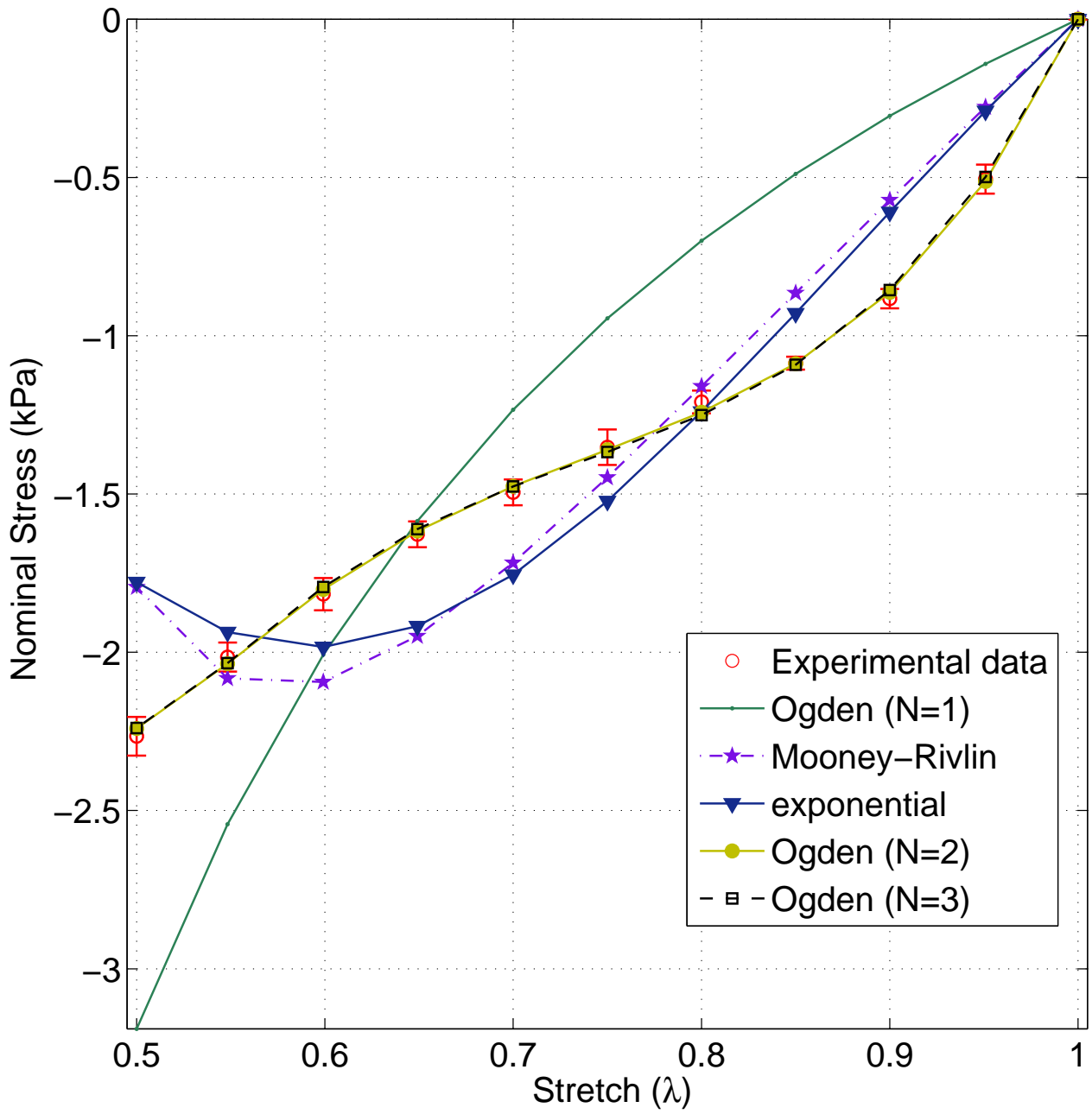


Figure 4: Data A: Comparison of Mooney-Rivlin, exponential and Ogden model fits.

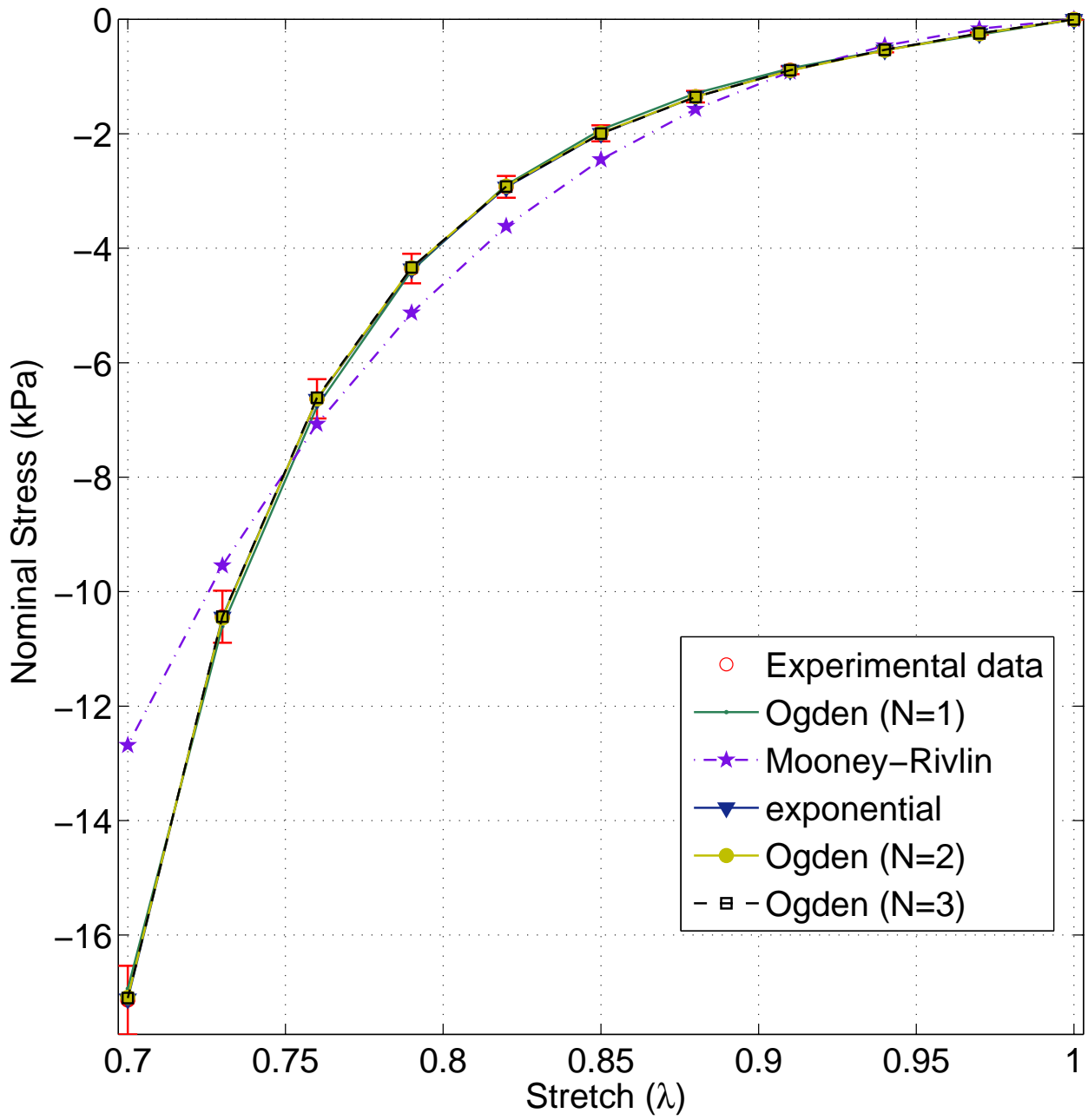


Figure 5: Data B: Comparison of Mooney-Rivlin, exponential and Ogden model fits.

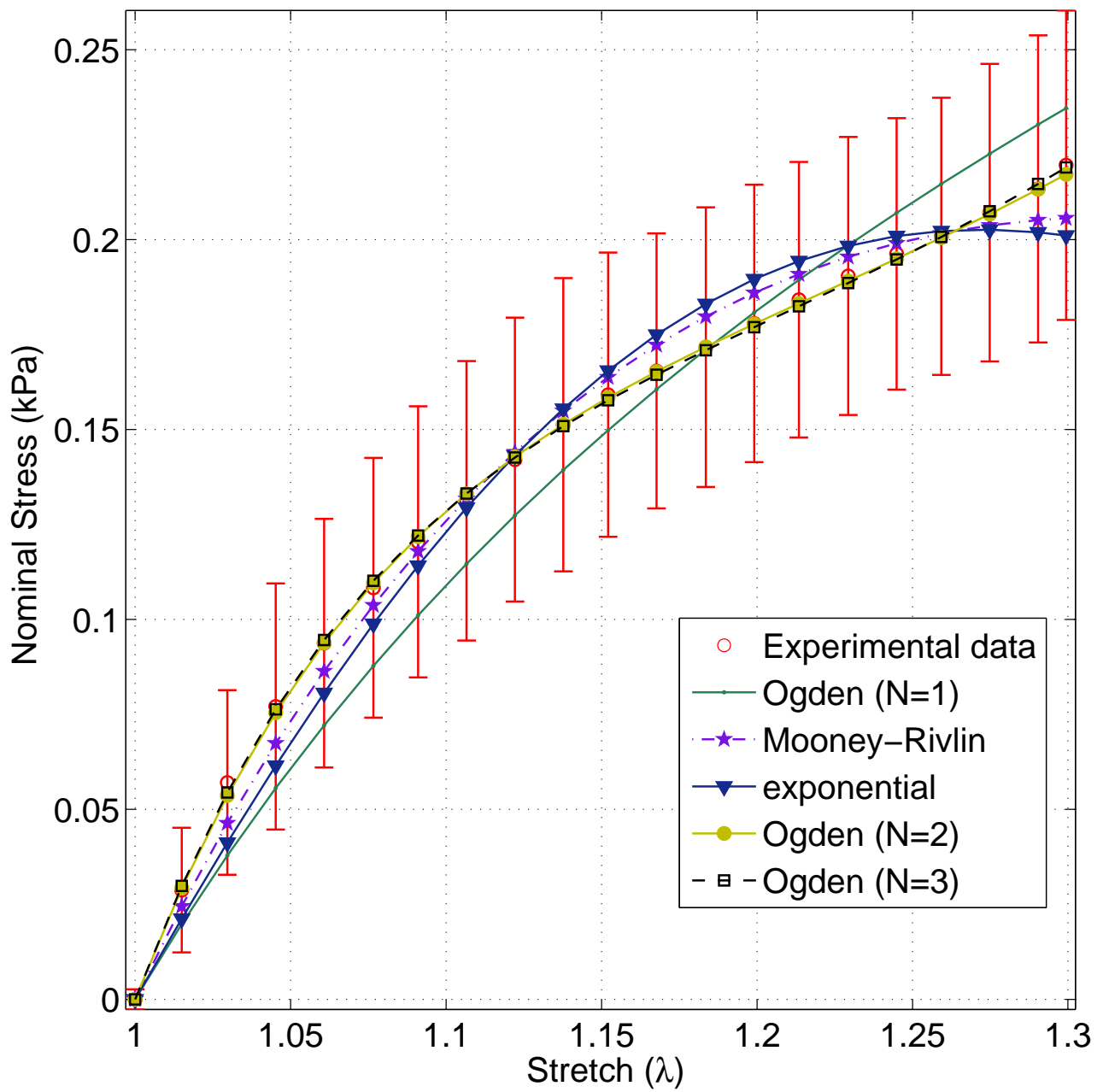


Figure 6: Data C: Comparison of Mooney-Rivlin, exponential and Ogden model fits.

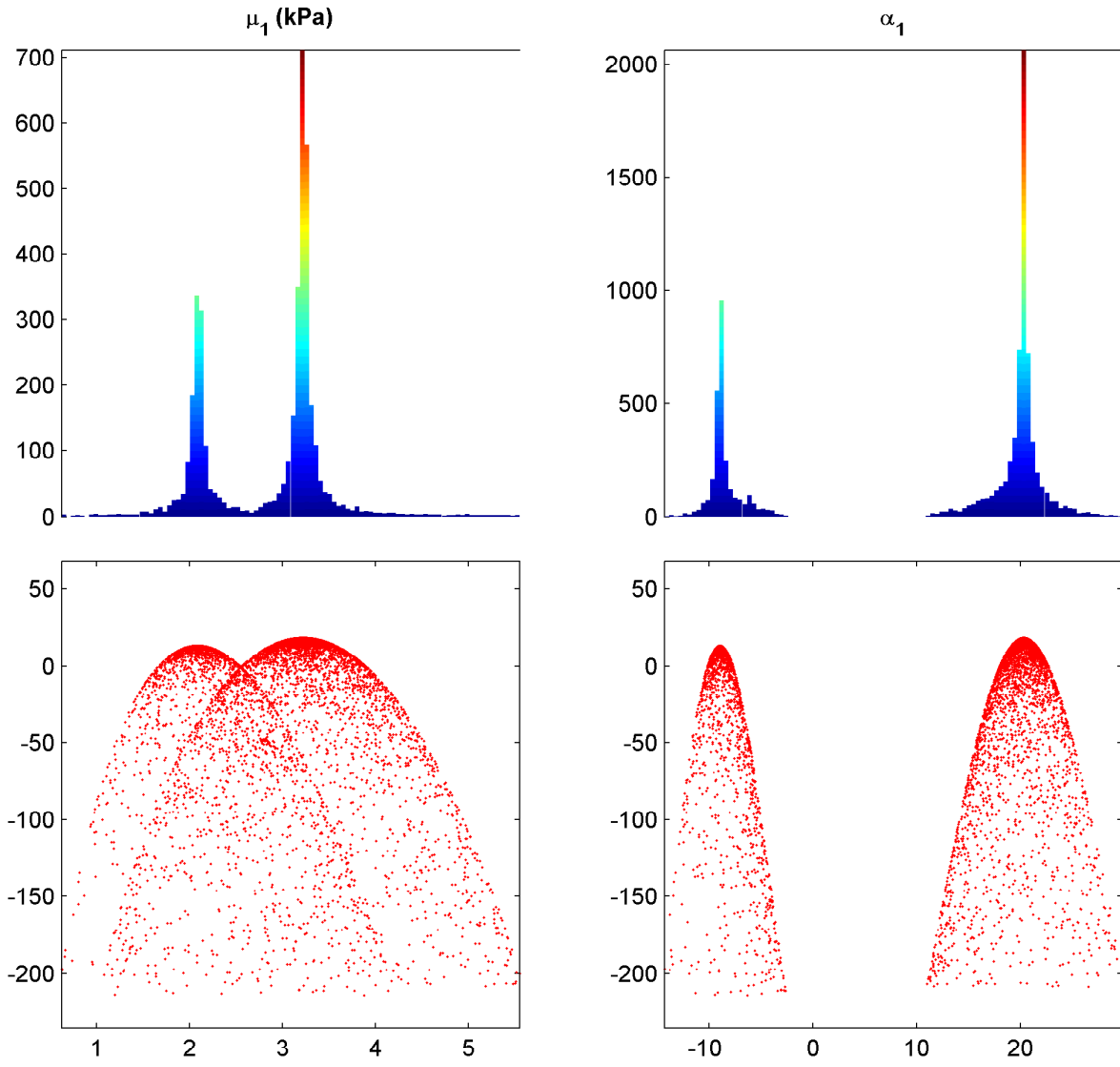


Figure 7: Data B: Log-likelihood distributions for the Ogden ( $N = 1$ ) model parameters.

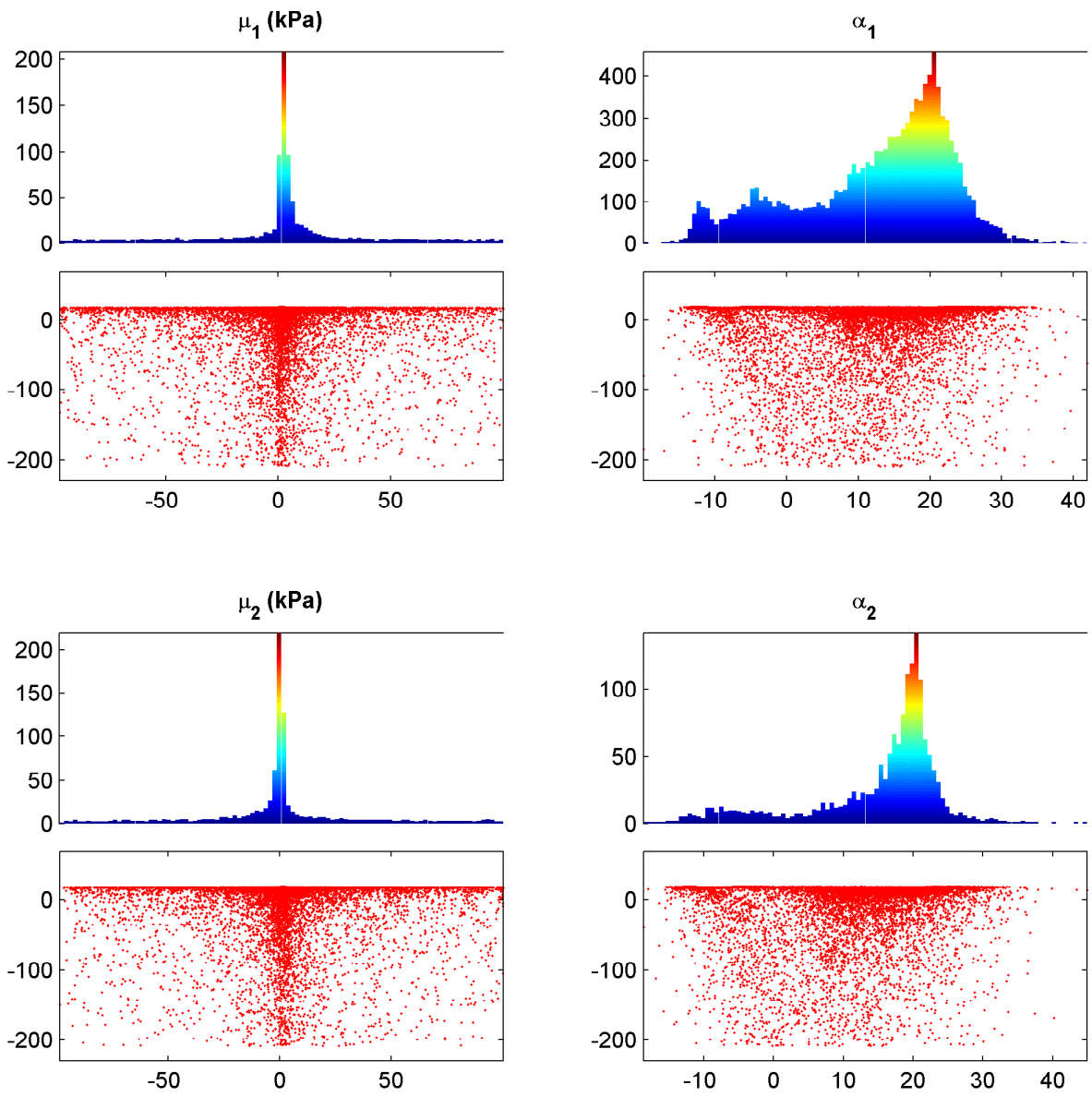


Figure 8: Data B: Log-likelihood distributions for the Ogden ( $N = 2$ ) model parameters.

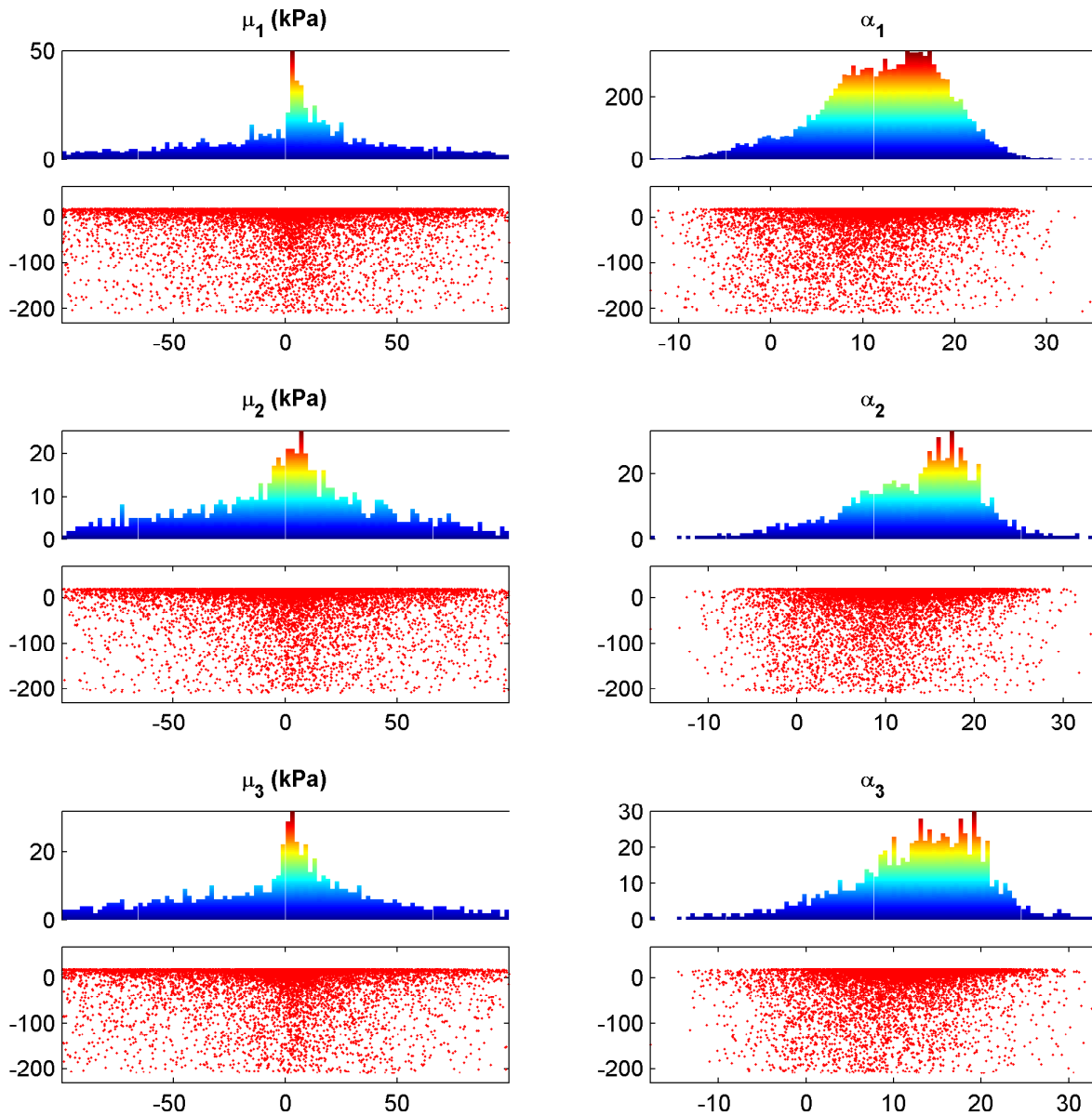


Figure 9: Data B: Log-likelihood distributions for the Ogden ( $N = 3$ ) model parameters.

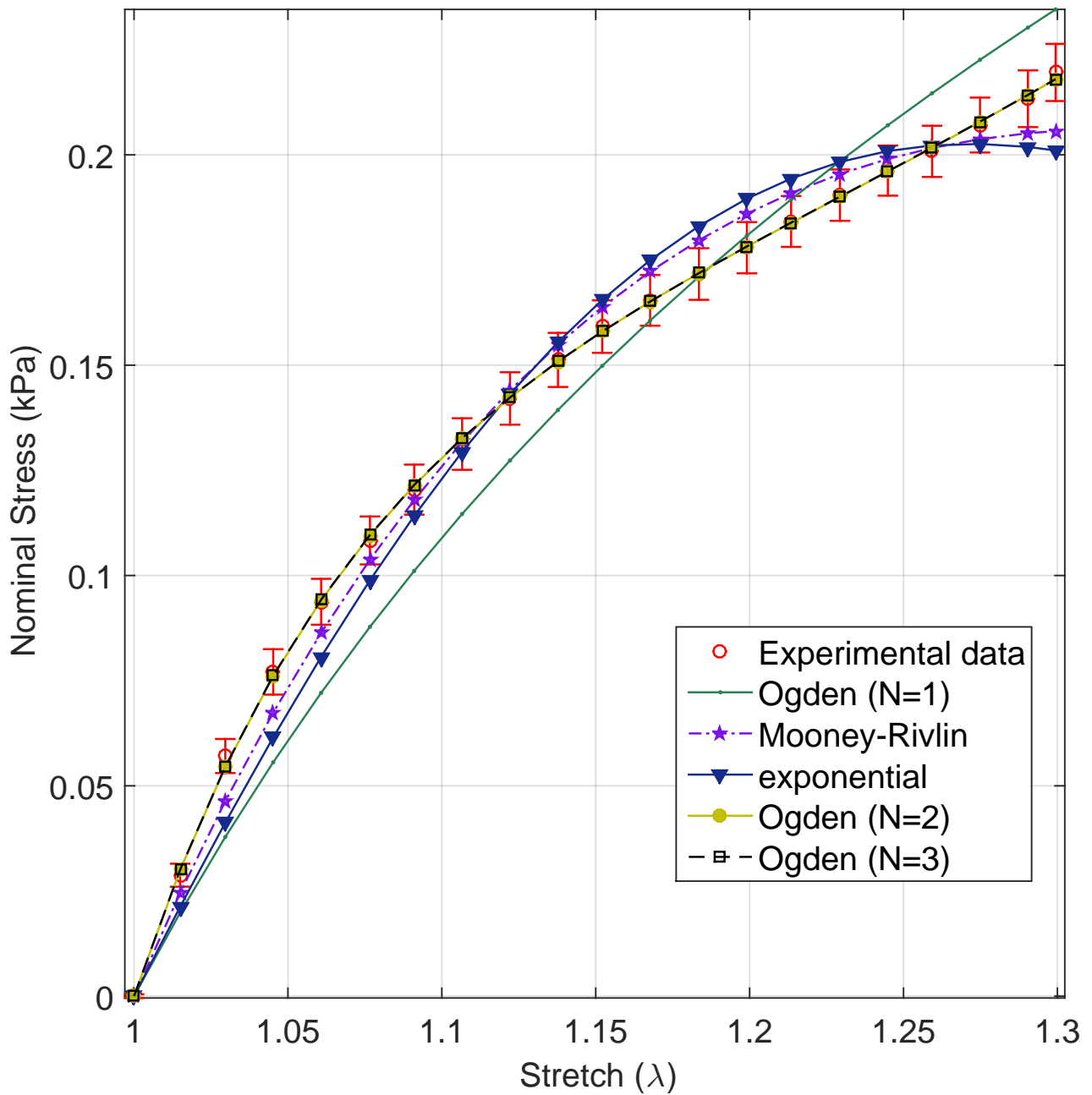


Figure 10: Data C with reduced noise: Comparison of Mooney-Rivlin, exponential and Ogden models fits.

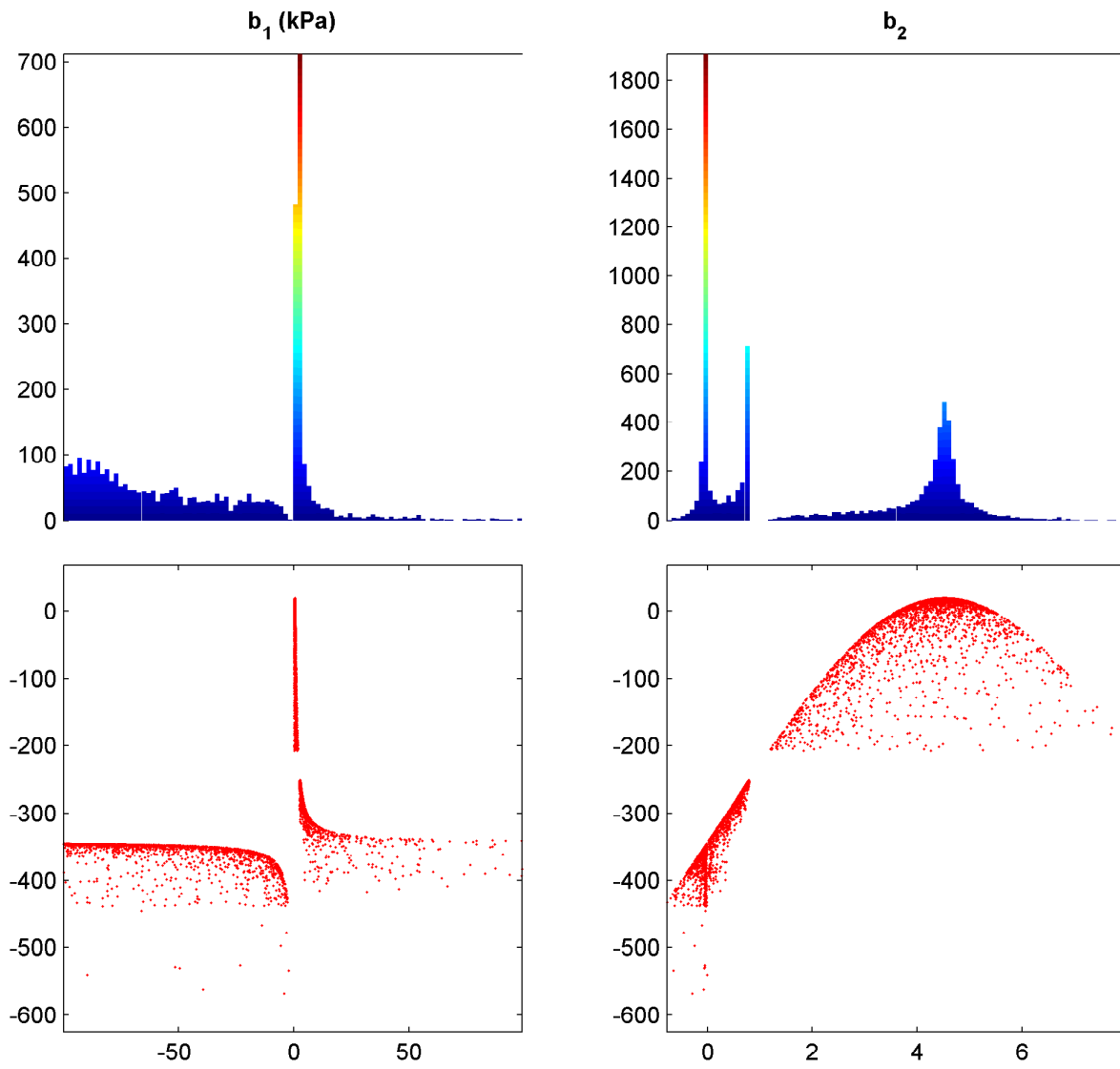


Figure 11: Data B: Log-likelihood distributions for the exponential model parameters.

$2 \log_e(B_{ab})$	$B_{ab}$	Evidence against model $M_b$	
0 to 2	1 to 3	Not worth more than a bare mention	Class 1
2 to 6	3 to 20	Substantial	Class 2
6 to 10	20 to 150	Strong	Class 3
> 10	> 150	Decisive	Class 4

Table 1: Jeffreys Scale, from [11].

	Data A	Data B	Data C
Material	agarose hydrogel	bovine liver	porcine brain
Testing Mode	unconfined compression	no-slip uniaxial compression	uniaxial tension
Strain Range	0 – 50%	0 – 30%	0 – 30%
Strain Rate	0.01/ <i>s</i>	0.04/ <i>s</i>	0.01/ <i>s</i>
Noise Level	low	low	high
Source	Billade [49]	Roan & Vemaganti [1]	Rashid et al. [51]

Table 2: Experimental data used in the study.

Material model	Data A		Data B		Data C	
	Uniform Prior	Gaussian Prior	Uniform Prior	Gaussian Prior	Uniform Prior	Gaussian Prior
Mooney-Rivlin	-184.537	-184.537	-40.256	-40.256	54.508	54.508
Exponential	-136.631	-136.631	19.415	19.415	53.968	53.968
Ogden ( $N = 1$ )	-942.329	-942.329	18.332	18.332	53.029	53.029
Ogden ( $N = 2$ )	30.931	30.929	19.376	19.403	54.897	54.898
Ogden ( $N = 3$ )	31.280	31.083	19.407	19.411	54.899	54.899

Table 3: The effect of the prior: Maximum of the log-likelihood function determined by the Bayesian approach.

Material model	Data A		Data B		Data C	
	Uniform Prior	Gaussian Prior	Uniform Prior	Gaussian Prior	Uniform Prior	Gaussian Prior
Mooney-Rivlin	-202.836 $\pm$ 0.066	-203.261 $\pm$ 0.067	-53.109 $\pm$ 0.054	-53.558 $\pm$ 0.055	39.385 $\pm$ 0.056	39.046 $\pm$ 0.060
Exponential	-153.915 $\pm$ 0.064	-154.398 $\pm$ 0.065	3.525 $\pm$ 0.061	3.234 $\pm$ 0.062	39.844 $\pm$ 0.056	39.844 $\pm$ 0.055
Ogden ( $N = 1$ )	-958.146 $\pm$ 0.061	-958.567 $\pm$ 0.062	5.778 $\pm$ 0.053	5.315 $\pm$ 0.056	41.721 $\pm$ 0.051	41.021 $\pm$ 0.053
Ogden ( $N = 2$ )	1.046 $\pm$ 0.083	1.411 $\pm$ 0.085	1.740 $\pm$ 0.062	0.902 $\pm$ 0.064	37.827 $\pm$ 0.062	36.973 $\pm$ 0.064
Ogden ( $N = 3$ )	-3.534 $\pm$ 0.086	-4.358 $\pm$ 0.085	-0.771 $\pm$ 0.067	-0.22 $\pm$ 0.069	34.951 $\pm$ 0.068	33.466 $\pm$ 0.070

Table 4: The effect of the prior: Marginal likelihood (Evidence) value determined by the Bayesian approach.

Data A		Data B		Data C	
Bayes Factor	Class	Bayes Factor	Class	Bayes Factor	Class
$\log_e(B_{O2-MR}) = 203.882$	Class 4	$\log_e(B_{O1-MR}) = 58.887$	Class 4	$\log_e(B_{O1-MR}) = 2.3360$	Class 2
$\log_e(B_{O2-EX}) = 154.961$	Class 4	$\log_e(B_{O1-EX}) = 2.2530$	Class 2	$\log_e(B_{O1-EX}) = 1.877$	Class 2
$\log_e(B_{O2-O1}) = 959.192$	Class 4	$\log_e(B_{O1-O2}) = 4.0380$	Class 3	$\log_e(B_{O1-O2}) = 3.8940$	Class 3
$\log_e(B_{O2-O3}) = 4.580$	Class 3	$\log_e(B_{O1-O3}) = 6.5490$	Class 4	$\log_e(B_{O1-O3}) = 6.770$	Class 4

Table 5: Bayes factors for the various datasets (MR: Mooney-Rivlin, EX:Exponential, O1: Ogden ( $N = 1$ ), O2: Ogden ( $N = 2$ ), O3: Ogden ( $N = 3$ ))

	Data A		Remarks
	Bayes factor	log-likelihood	
Rank 1	Ogden ( $N = 2$ )	Ogden ( $N = 3$ )	(a) Fits to data good for Ogden ( $N = 2, 3$ )
Rank 2	Ogden ( $N = 3$ )	Ogden ( $N = 2$ )	(b) The likelihood surface is flat for Ogden ( $N = 3$ ),
Rank 3	exponential	exponential	indicating over-fitting
Rank 4	Mooney-Rivlin	Mooney-Rivlin	
Rank 5	Ogden ( $N = 1$ )	Ogden ( $N = 1$ )	

Table 6: Data A: Model ranks based on Bayes factor and maximum log-likelihood

	Data B		Remarks
	Bayes factor	log-likelihood	
Rank 1	Ogden ( $N = 1$ )	exponential	(a) Fits to data good for exponential, Ogden ( $N = 1, 2, 3$ ) (b) The likelihood surface is flat for Ogden ( $N = 2, 3$ ) (c) exponential: probability mass with high likelihood is smaller than with Ogden ( $N = 1$ )
Rank 2	exponential	Ogden ( $N = 3$ )	
Rank 3	Ogden ( $N = 2$ )	Ogden ( $N = 2$ )	
Rank 4	Ogden ( $N = 3$ )	Ogden ( $N = 1$ )	
Rank 5	Mooney-Rivlin	Mooney-Rivlin	

Table 7: Data B: Model ranks based on Bayes factor and maximum log-likelihood

	Data C		Remarks
	Bayes factor	log-likelihood	
Rank 1	Ogden ( $N = 1$ )	Ogden ( $N = 3$ )	(a) Fits to data good for Ogden ( $N = 2, 3$ )
Rank 2	exponential	Ogden ( $N = 2$ )	(b) The likelihood surface is flat for Ogden ( $N = 2, 3$ )
Rank 3	Mooney-Rivlin	Mooney-Rivlin	(c) Under-fitting model preferred over over-fitting model
Rank 4	Ogden ( $N = 2$ )	Exponential	(d) The right model balancing goodness of fit and
Rank 5	Ogden ( $N = 3$ )	Ogden ( $N = 1$ )	model complexity not in the candidate set

Table 8: Data C: Model ranks based on Bayes Factor and maximum log-likelihood

Material model	Max log-likelihood	log-evidence
Mooney-Rivlin	77.979	$59.409 \pm 0.066$
Exponential	58.528	$40.776 \pm 0.064$
Ogden ( $N = 1$ )	24.733	$9.843 \pm 0.058$
Ogden ( $N = 2$ )	92.068	$69.093 \pm 0.073$
Ogden ( $N = 3$ )	92.085	$66.589 \pm 0.077$

Table 9: Maximum of the log-likelihood function and evidence with experimental variance one-sixth of the original for Data C.