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Uncertainty Quantification for Nonparametric Estimation of Probability Measures and Delay Differential Equations Driven by Colored Noise

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14. ABSTRACT
We have continued our joint investigations on the identification of thermal degradation using probabilistic models in reflectance spectroscopy. These were carried in continued collaboration with scientists at AFRL (Materials State Awareness & Supportability Branch, Air Force Research Lab, WPAFB 45433, USA) lead by Amanda K. Criner. Reflectance spectroscopy obtained from a thermally treated silicon nitride carbon based ceramic matrix composite was used to quantity the oxidation products SiO2 and SiN.Our estimation results indicate a distinguishable increase in the SiO2 present in the samples which were heat treated for 100 hours compared to 10 hours.
In our consideration of several other problems of interest to DOD, we discuss two other problems where aggregate data is often mistreated as individual data. The problems, PBPK modeling and Food Chemistry Modlels and possible improvements in the associated inverse problems are discussed and summarized in separate papers.We propose in [11] a novel method which accounts for inter-individual variability in experiments where only unidentified individual data is available. Both parametric and nonparametric methods for estimating the distribution of parameters which vary among individuals are developed. These methods are illustrated using both simulated data, and data taken from a physiological experiment. Taking the approach outlined in [11] results in more accurate quantification of the uncertainty attributed to interindividual variability.

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AFOSR 2015-2018 FINAL REPORT-SUMMARY

When estimating parameters using noisy data, uncertainty quantication methods provide a way to in-vestigate the confidence one has in the parameter estimates, as well as to obtain information on the possible dependence of parametric estimators on one another. In [1], we consider uncertainty quantication techniques that allow visualization of the distributions of these parameter estimators for evidence of possible correlation. We consider three mathematical models (the logistic curve, the Richards curve, and the spring equation), which permit multiple parametrizations, and compare the corresponding parameter estimators for possible dependence/independence. The uncertainty quantification techniques we employ include the correlation coefficients, asymptotic as well as exact confidence regions or ellipsoids, and Monte Carlo plots generated by the DRAM algorithm.

We have continued [4, 7] our joint investigations on the identification of thermal degradation of composite materials using probabilistic models in reflectance spectroscopy. These were carried in continued collaboration with scientists at AFRL (Materials State Awareness & Supportability Branch, Air Force Research Lab, WPAFB 45433, USA) lead by Amanda K. Criner where a member of our team (J. Catenacci) spent a summer internship in 2015. Reflectance spectroscopy obtained from a thermally treated silicon nitride carbon based ceramic matrix composite was used to quantity the oxidation products SiO_2 and SiN. The data collection is described in detail in [4] in order to point out the potential biasing present in the data processing. A probability distribution is imposed on select model parameters, and then non-parametrically estimated. A non-parametric estimation is chosen since the exact composition of the material is unknown due to the inherent heterogeneity of ceramic composites. The probability distribution is estimated using the Prohorov Metric Framework (PMF) in which the infinite dimensional optimization is reduced to a finite dimensional optimization using an approximating space composed of linear splines. A weighted least squares estimation is carried out, and uncertainty quantification is performed on the model parameters, including a piecewise asymptotic confidence band for the estimated probability density. Our estimation results indicate a distinguishable increase in the SiO_2 present in the samples which were heat treated for 100 hours compared to 10 hours.

In [7] we consider the case of non-parametric estimation of a probability measure under the Prohorov metric framework in a least squares problem. It is demonstrated that the gradient computation can be reduced by exploiting the linearity of the coefficients to be estimated which appear in the approximation schemes under the PMF. For individual models the number of forward solves of the underlying model is reduced from O(N^2) to O(N), where N is the number of elements in the approximation. Due to the use of the exact partial derivatives in computing the gradient, there is no truncation error present from a finite differencing of the objective function. An example using a Sinko-Streifer model with aggregate data is discussed in [7] and the expected linear increase in cpu time as N increases was observed. For aggregate models the reduction of computational expense in computing the gradient of the objective function is not as straight forward. This is due directly to the fact that the model depends explicitly on the probability measure for aggregate models. However, we still can reduce the number of evaluations of the probability measure kernel function from O(N^2) to O(N). The practical degree to which any speed up can be obtained in the inverse problem depends directly on the complexity of the kernel function. If it is relatively cheap to evaluate, then the speed up may be negligible, even though we have reduced the number of evaluations. However, if the kernel function is costly to evaluate, then the speed up may be significant. We demonstrated this in [7] with an example arising in an application using reflectance spectroscopy, and the cpu time was observed to have the expected linear behavior.

In our consideration of several other problems of interest to DOD, we mention two problems where aggregate data is often mistreated as individual data. The problems and possible improvements in the associated inverse problems are discussed in [11] and [12] respectively, and summarized briefly here.

In physiological experiments, it is common for measurements to be collected from multiple subjects. Often it is the case that a subject cannot be measured or identified at multiple time points (referred to as unidentified individual data in [11] but often referred to as aggregate population data [Banks,Hu,Thompkins, *Modeling and Inverse Problems in the Presence of Uncertainty*, 2014, Chapter 5]). Due to a lack of alternative methods, this form of data is typically treated as if it is collected from a single individual. This assumption leads to an overconfidence in model parameter values and model based predictions. We propose in [11] a novel method which accounts for inter-individual variability in experiments where only unidentified individual data is available. Both parametric and nonparametric methods for estimating the distribution of parameters which vary among individuals are developed. These methods are illustrated using both simulated data, and data taken from a physiological experiment. Taking the approach outlined in [11] results in more accurate quantification of the uncertainty attributed to inter-individual variability.

In the second application we analyze in [12] a quasi-chemical kinetic food chemistry model in the context of a parameter estimation problem using available experimental data sets. For many of the data sets the dynamics are quite simplistic and we show that the quasi-chemical model (QCM) is over parameterized in these cases. This results in larger uncertainty in the estimated parameters and is some cases instability in the inverse problem. We illustrate methods for reducing the uncertainty present in the estimated model parameters. We first consider a model reduction technique where subsets of the QCM parameters are fixed at nominal values and hypothesis testing is used to compare the nested models. An orthogonal decomposition of the sensitivity matrix is used to guide the choice of which parameters are fixed. Additionally, simple surrogate models are developed to compare to the QCM. In most cases one of the surrogate models is able to fit the data nearly as well as the QCM model while significantly reducing the uncertainty in the model parameters.

Much of the literature on inverse problem uncertainty depends substantially on sensitivity functions and their computation. In [5] we investigate the complex-step method as applied to compute sensitivities with respect to model "parameters" for several types of examples. We first consider time delayed differential equations (DDEs) whose sensitivities are known to have lack of smoothness or even discontinuities with respect to parameters such as the delays. The second type of "parameter sensitivity" we consider is that of solutions to partial differential equations (PDEs) with respect to boundary conditions which again may not possess smoothness. These sensitivities are fundamental in any type of boundary control formulation such as those motivated in [5]. Our main focus in [5] is to evaluate the so-called "complex-step methods" for computing such sensitivities. This is of interest since the complex-step method was derived based on the Cauchy-Riemann equations for analytic complex functions. Our computational findings are compared to those using the standard chain rule-based sensitivity differential equations which can be rigorously developed even for derivatives possessing much less regularity than analyticity. Our findings suggest that the complex-step methods are in very good agreement with the usual sensitivity equation results up to some critical step size we call hcrit. They can offer significant savings in computational costs for problems driven by complicated dynamical systems with reasonable parameter size.

In [15] we continued our investigation of the ***complex-step derivative approximation technique to compute sensitivities*** for delay differential equations (DDEs) with non-smooth (discontinuous and even distributional) history functions. We knew from previous efforts that such delay systems could easily generate solutions that failed the traditional analyticity requirements for the complex-step to be used. In the studies we sought to reveal the sort-comings of the method. In the process we discovered that the method could be established under *far weaker asssumptions than known in the literature*. In particular we found that the standard expression can be obtained by approximating a C^2 function *f(q)* with a complex variable using a 2nd order *Taylor* expansion with remainder:

$$f\ (q + ih) \approx\ f(q) + ih\, f'(q) + R(q)$$

where $R(q)$ is $O(h^2)$. Taking the imaginary parts of both sides and dividing by *h* gives

$$f'(q) \approx\ \frac{Im[f(q+ih)]}{h} + O(h^2).$$

Terms of order h^2 and higher can be ignored because the step size *h* can be chosen up to machine precision. Thus the *complex-step* derivative is given above with a truncation error $E_t(h) = \frac{h^2}{6} f^{(3)}(q)$. The method is accurate down to a specific step size we call h_{crit}. Below h_{crit}, underflow occurs and the approximation becomes useless. The derivative estimate constitutes a big advantage over the finite-difference approach to sensitivities. First, it is applicable for problems with less smoothness than analyticity (e.g., only C^2 functions of the parameters). Moreover, the finite-difference approximation is subject to *subtractive error* due to the differencing operation. On the other hand, the accuracy of the complex-step estimates is only limited by the numerical precision of the algorithm that evaluates the function *f*.

We have very successfully used this approach in our subsequent efforts [24,26] on studies for systems as a precusor **to *control of fluid-structures dynamics*** as well as in biological/ecological and psychological systems [16,18,28]. In the studies in [24,26], we consider poro-elastic and poro-visco-elastic models inspired by problems in medicine and biology. Poro-elastic systems have been used extensively in modeling fluid flow in porous media in petroleum and earthquake engineering. More recently, they are frequently used to model fluid flow through biological tissues (elastin, collagen) , cartilages, and bones with our primary interest raised by applications to adaptive control of glucoma. We performed sensitivity analysis on the solutions of these fluid-solid mixtures problems with respect to the imposed boundary data, which are the main drivers of the system. Moreover, we compared the results obtained in the elastic case vs. viscoelastic case, as it is known that structural viscosity of biological tissues decreases with age and disease. Sensitivity analysis is the first step in identifying important parameters to control or use as control terms in these poro-elastic and poro-visco-elastic models, which is our ultimate goal.

Again, we have continued collaboration with scientists at AFRL (Materials and Manufacturing Directorate, Air Force Research Laboratory WPAFB 45433, USA) led by Amanda K. Criner on efforts with iceramic matrix composites. We received **new data** in Dec 2016 on SiC_f/SiC composites and have been analysizing this data in the latter half of the reporting period. Banks and his student, Rebekah White, spent two days at WPAFB in early March, 2017, and Criner visted NCSU in late May at same time our Argentine co-workers (D. Rubio and colleagues) were visitng. Prior to this year we had been using advanced techniques (probability distributions estimated using the Prohorov Metric Framework (PMF) in which the infinite dimensional optimization is reduced to a finite dimensional optimization using an approximating space composed of linear splines) in investigations on the identification of thermal degradations using probabilistic models in reflectance spectroscopy in response to frequency sweeps. Our findings to date suggest with this increasing sophisticated data we should expand our efforts by using *absorption* and *transmission* properties of the materials along with the refection spectroscopy. Our close collaborations with WPAFB on non-invasive and non-destructive interrogation techniques are continuing.

In a series of efforts [19,21], we considered model comparison techniques for three different classes of ***stochastic models***: *continuous time Markov chains* (CTMC), *stochastic differential equations* (SDE), and *random differential equations* (RDE). For *nested models*, we extended the statistically-based ideas and techniques developed earlier by Banks and Fitzpatrick for deterministic differential equation models to these three types of stochastic systems. We illustrated the ideas in the context of examples with simulated data and then applied the ideas to inverse problems for growth data from algae experiments. We considered in [21] two distinct techniques for estimating random parameters in *random differential equation* (RDE) models. In one approach, the solution to an RDE is represented by a collection of solution trajectories in the form of sample deterministic equations. In a second approach we employed pointwise equivalent stochastic differential equation (SDE) representations for certain classes of RDEs. Each of the approaches is tested using deterministic model comparison techniques for a logistic growth model which is viewed as a special case of a more general Bernoulli growth model. We demonstrated efficacy of the preferred method with experimental data using algae growth model comparisons. In a related effort for non-nested systems [25], we explained the use of the Akiake Information Criterion and its related model comparison indices (usually derived for *maximum likelihood estimator inverse problem formulations*) for use with *least squares* (ordinary, weighted, iterative reweighted weighted or ”generalized” least squares) based inverse problem formulations. The ideas are illustrated with several examples of interest in biology/ecology and the environmental sciences .

In [43,45] we considered nonparametric estimation of probability measures for parameters in problems where only aggregate (population level) data are available. We considered an existing computational method for the ordinary differntial eqaution syatem estimation problems we have developed over the past several decades . Theoretical results were then presented which establish the existence and consistency of very general (ordinary, generalized and other) least squares estimates and estimators for the measure estimation problem with specific application to *random Partial Differential equations and random Delay Differential equations.*

Motivated by another class of problems where only aggregate data is available, we have pursued joint inviaetigations with a team of mechanical engineers at NCSU [33,39] in problems involving bone density and porosity in animals and humans. Our findings will have importance in the study of osteoporosis. Osteoporosis changes the micro-structure of both cortical and trabecular bone which leads to fragility fractures, higher morbidity and mortality, and reduction of life expectancy. Because it constitutes 80 percent of the human skeleton, cortical bone supports the main load of the body and largely contributes to the skeletal mechanical competence. The microarchitecture of cortical porosity impacts the macroscopic mechanical properties of cortical bone, and is affected by osteoporosis. It is therefore highly relevant to develop methods for the quantitative assessment of the micro-architecture of cortical porosity, and we hypothesize that tracking the micro-structural changes in cortical bone could benefit the early stage diagnosis of osteoporosis and may enable treatment monitoring.

In [33] a mathematical model to predict the ultrasonic attenuation coefficient as a function of frequency in cortical bone is proposed, and the effects of micro-architectural changes on model parameters are studied. Spectroscopy was performed in numerical finite differences time domain simulations to study the individual effects of pore diameter on ultrasonic attenuation. The attenuation coefficient was calculated by measuring the wave amplitude of the wave propagated in simulated bone slabs. Data obtained from numerical simulations show an acceptable match with the proposed model, and the model parameters varied consistently with increasing pore diameter in the cortical bone slabs. Results of this research indicate the potential of a mathematical model to predict the dispersion of attenuation in cortical bone as a function of frequency, pore size and pore density.

In [39] we propose a phenomenological power law model to describe the attenuation of ultrasonic waves in cortical bone. We use data generated using a finite-difference, time domain (FDTD) numerical simulation. We fit this phenomenological model to the simulated data by optimizing parameters under an ordinary least squares (OLS) framework. Local sensitivity analysis is then performed on the resulting parameter estimates in order to determine to which parametes the model are most sensitive. We find that the sensitivity of the model to various parameter estimates depends on the micro-architectural parameters, pore diameter (ϕ) and pore density (ρ). In order to otain a sense for how confidently we are able to estimate model parameters, we calculate 95% confidence intervals for these estimates. In doing so, we establish the ability to estimate model-sensitive parameters with a high degree of confidence. Being able to accurately estimate model parameters from which we hope to infer micro-architectural ones, will allow us to determine pore density and diameter via an inverse problem given real or simulated ultrasonic data. Our efforts on developing more physically-based mathematical models is continuing.

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Abstract

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Finally in [43,45] we have extended our general theory for treatment of aggregate data problems to random PDEs and random DDEs. With the co-investigatiors from mechical engineering we have in [33,39] investigated problems related to cortial bone density and its changes over time which are models involving aggregate data experiments.

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New discoveries, inventions, or patent disclosures:

Do you have any discoveries, inventions, or patent disclosures to report for this period?

No

Please describe and include any notable dates

Do you plan to pursue a claim for personal or organizational intellectual property?

Changes in research objectives (if any):

None

Change in AFOSR Program Officer, if any:

None

Extensions granted or milestones slipped, if any:

None

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

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Appendix Documents

2. Thank You

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