SAND2018-2265C

Dealing with nuisance parameters in Bayesian model calibration

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Abstract: We consider the problem of physical parameter estimation by coupling experimental data with computational simulations. The Bayesian Model Calibration (BMC) framework accommodates a wide variety of uncertainties, including model misspecification and is thus a useful tool for solving these inverse problems. In the presence of a high-dimensional vector of *nuisance parameters*, this problem is often poorly identified. We propose statistical methodologies backed by rigorous mathematical theory for calibrating physical parameters in precisely this situation. First, we consider *regularization,* the specification of hierarchical shrinkage priors on the nuisance parameters in an effort to preserve measurement uncertainty structure and to avoid over-fitting. Secondly, we consider *modularization,* an alternative to the full Bayesian approach which eliminates *contamination* of the physical parameters via the difficult-to-learn nuisance parameters. Finally, these methods are applied in a dynamic materials setting to produce inferences on the material properties of tantalum.

Dynamic material property calibration

Objective: By coupling experimental and simulated velocity traces, parameters of the tantalum equation of state (EOS) are estimated. The EOS of a material describes the pressure-volume-temperature relationship.

Experimental setup (Figure 1)**:** Massive electrical currents associated with strong time-dependent magnetic fields are treated as boundary conditions resulting in a stress wave propagating through the system as a function of time. Velocity of the stress wave is measured at the interface of the Ta sample and LiF window and can be compared to simulated velocities.

Uncertainties: Time and velocity are measured with error and an emulator is used as a proxy to the computer model. Bulk modulus and its pressure derivative (B_0 and B_0') are the physical parameters of interest. Nuisance parameters include Ta density, magnetic field scaling and thickness of the Al and Ta. The parameters describing scaling and thickness may vary across experiments, yielding 28 nuisance parameters.

Data (Figure 2)**:** The experimental data consists of 9 velocity traces. For each experiment, Latin Hypercube Sampling over the 6 inputs was used to simulate 5,000 velocity curves from the computer model. These 45,000 simulated velocity traces were then used to build an emulator for the computer model.

Figure 1: Experimental setup

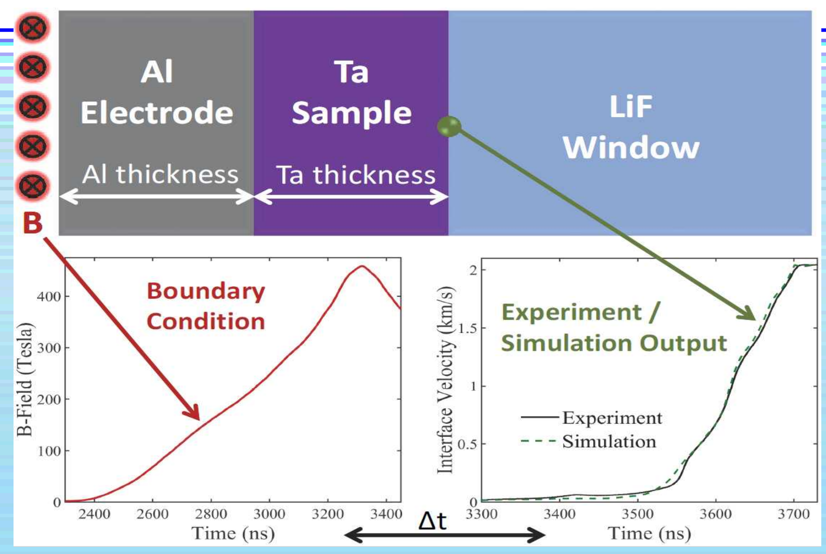
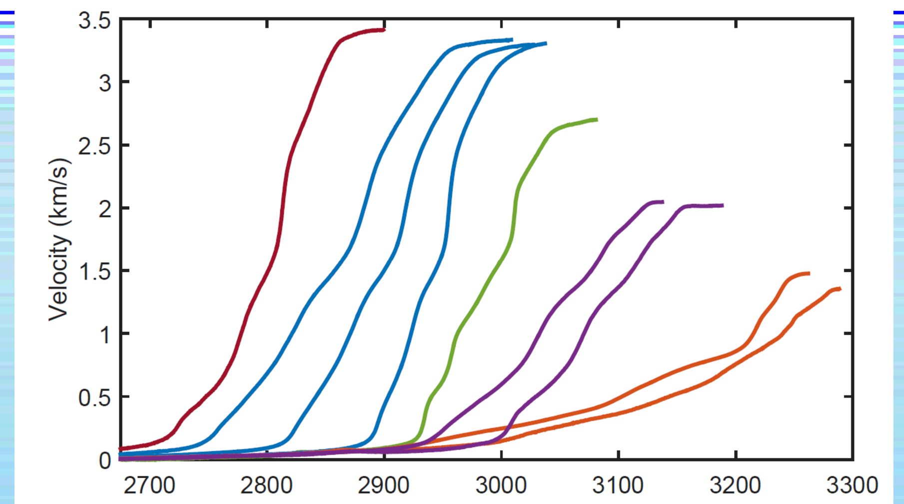


Figure 2: Measured velocity traces



Regularization vs Modularization

BMC model: (Kennedy and O'Hagan) For experiment j, the measured velocity y_{ij} is modeled as a function of time x_{ij} and the unknown parameters θ_j.

$$y_{ij} = \eta(x_{ij}, \theta_j) + \delta_j(x_{ij}) + \epsilon_{ij}$$

$$\delta_j \sim GP(0, \Sigma_j) \quad \epsilon_{ij} \sim N(0, \sigma^2(x_{ij}))$$

For convenience, we partition the parameters as $\theta_j = (\boldsymbol{\alpha}, \boldsymbol{\gamma_j})$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$ are the physical parameters of interest, and $\boldsymbol{\gamma_j} = (\gamma_1, \gamma_{2j}, \gamma_{3j}, \gamma_{4j})$ are the experiment-dependent nuisance parameters.

Regularization: A model with such a large number of nuisance parameters will often be non-identifiable. In the presence of model misspecification, standard BMC will update the nuisance parameters incorrectly, resulting in biased estimates of the physical parameters. In *regularization*, we use the following hierarchical priors.

$$\gamma_{kj}|\mu_k \sim N(\mu_k, 1), \qquad \mu_k \sim N(0, J^{-1}), \qquad k = 2,3,4 \qquad j = 1,2, \ldots J$$

Where J=9 is the number of experiments.

Modularization: In some cases, we may be forced to accept that updating the nuisance parameters will lead to overfitting. This can result in biased estimates and underestimation of uncertainty for the parameters of interest. One option then is to mimic the forward propagation of uncertainty via modularization of the nuisance parameters by sampling their priors rather than updating.

Results

- *Note: These results were obtained setting $\gamma_{3j} = \gamma_{4j} = 0$ for all j.*
- We found that **Regularization** was numerically more stable for our application, but was otherwise similar to the standard BMC. Future work will examine the effects of priors which induce *shrinkage* and *sparsity* on the nuisance parameters.
- **Modularization** yields more uncertainty in the posterior distributions for the physical parameters. This effect is desirable if we believe that the model is mis-specified and may be overfitting. Future work will focus on improving the efficiency of the implementation.
- Figure 5 demonstrates that differences in *model discrepancy* due to different parameter values is primarily additive. Future work will look at this as a diagnostic tool for assessing independence between the model discrepancy and the parameters.

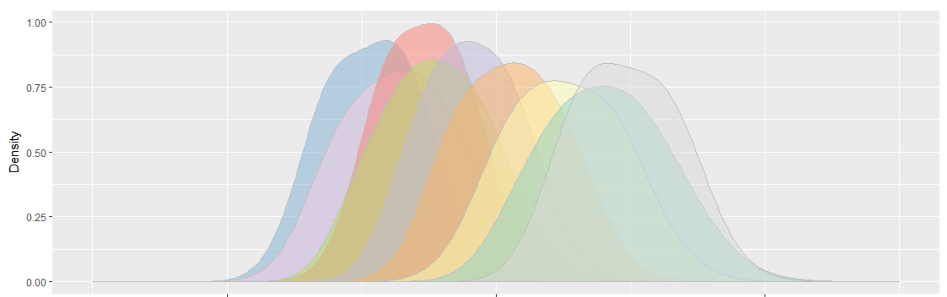


Figure 3: Posterior densities of the "scaling" nuisance parameters for each of the nine experiments under the hierarchical regularization prior.

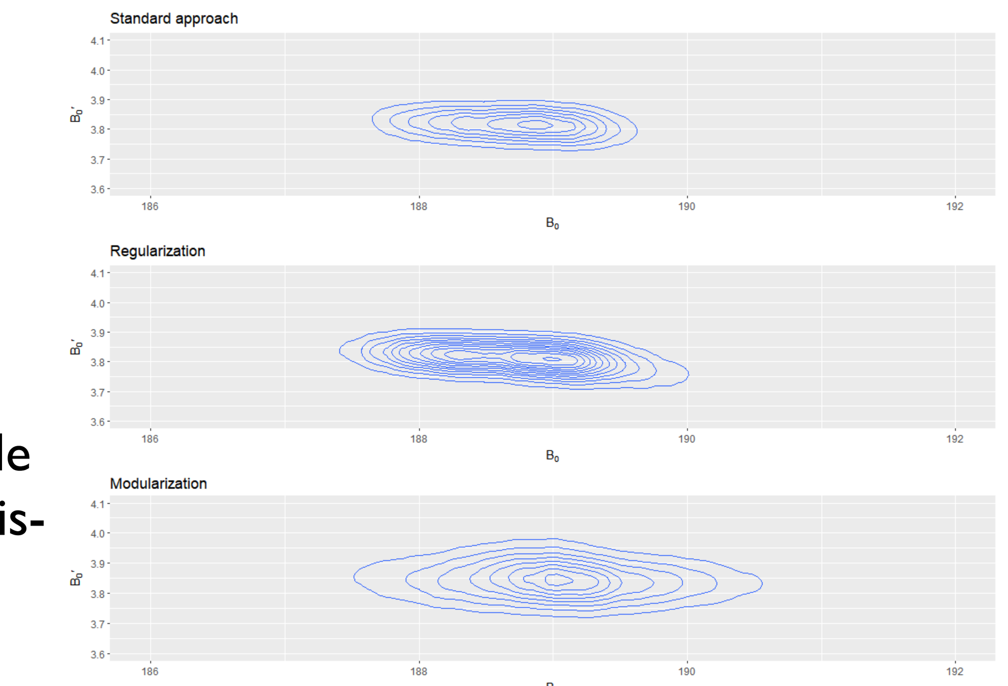


Figure 4: Posterior contours for the physical parameters of interest for each method.

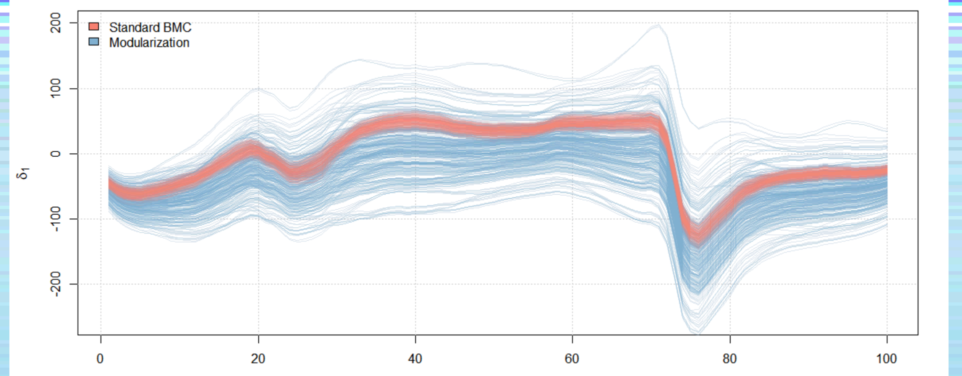


Figure 5: Estimates of the model discrepancy for experiment 1. Uncertainty in the parameters is propagated forward.

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