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Dealing with nuisance parameters in Bayesian model calibration

PRESENTED BY

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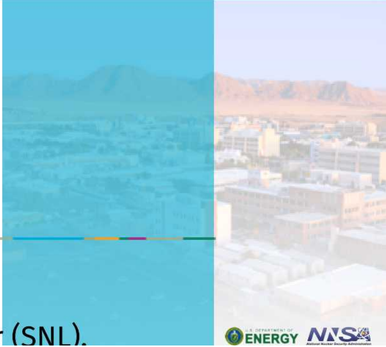

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Statement

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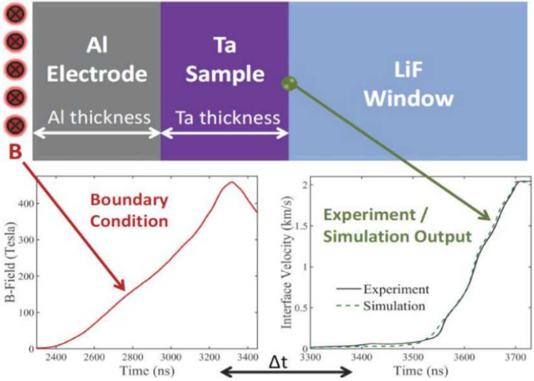
Background

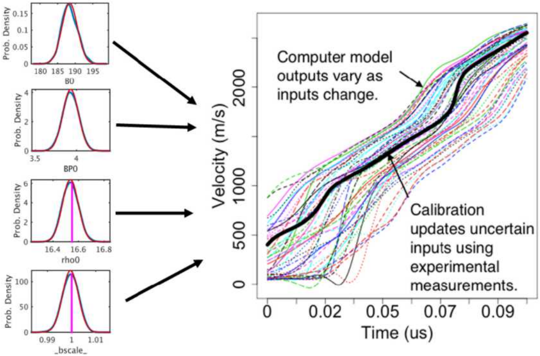
- **Dynamic material properties experiments**: access to the most extreme temperatures and pressures attainable.
- **Sandia National Labs Z-machine**: pulsed power driver that can deliver massive electrical currents over very short timescales (of the order of 60MA over $1\mu s$)).
- **Goal:** Understanding of material models at extreme conditions by coupling computational simulations with experimental data.
- **Parameters of interest are physical**: material properties with "true" value that is of interest.
- **Firstly**: Calibrate a well-understood model - two parameters of the equation of *state of tantalum*.

Experimental setup



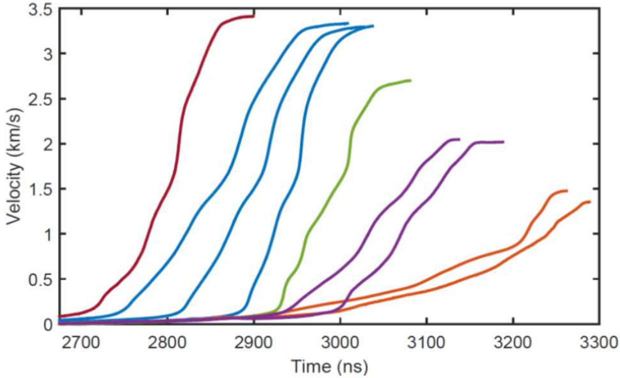
- "By coupling experimental and simulated velocity traces, parameters of the tantalum (Ta) equation of state (EOS) can be estimated".
- Massive electric currents treated as boundary conditions.
- Stress wave propagates thru system.

Calibration



- Uncertain inputs generate velocity curves using a computer model.
- Probability distributions look for ”agreement” of outputs and measurements.
- Bayesian framework is a natural in this context.

Challenge



- How to accurately estimate uncertainties?
- Calibration parameters have physical interpretation.
- Lots of *nuisance* parameters.

Our Framework

- Model the i^{th} observation in the j^{th} experiment as (Kennedy & O'Hagan 2001),

$$y(x_{ij}) = \eta(x_{ij}, \boldsymbol{\alpha}, \boldsymbol{\gamma}_j) + \delta(x_{ij}) + \epsilon_{ij}$$

- $\boldsymbol{\alpha}$ are the (unknown) values of the calibration parameters.
- $\boldsymbol{\gamma}_j$ unknown values of experimental uncertainties for experiment j.
- $y(x_{ij})$ is the observed velocity at time x_{ij}.
- $\eta(x_{ij}, \boldsymbol{\alpha}, \boldsymbol{\gamma}_j)$ is the computer model output at x_{ij}.
- $\delta(x_{ij}) \sim GP(\boldsymbol{\mu}_\delta, \boldsymbol{\Sigma}_\delta)$
- ϵ_{ij} are errors at x_{ij}.

Dynamic material property calibration

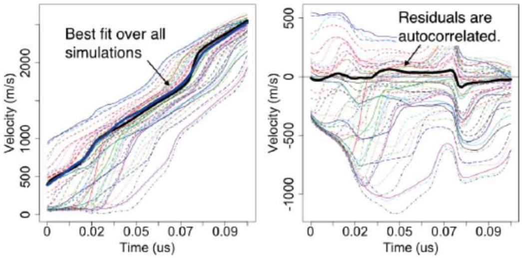
- BMC framework to obtain inference for two material properties of Tantalum.
- B_0 and B_0' are the Bulk modulus of tantalum and its pressure derivative.

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2) = (B_0, B_0')$$

- Four nuisance that may vary across $p = 9$ experiments
  - Tantalum density - γ_1
  - Magnetic field scaling - γ_{2j}, $j = 1, 2, \cdots 9$
  - Aluminum thickness- γ_{3j}, $j = 1, 2, \cdots 9$
  - Tantalum thickness - γ_{4j}, $j = 1, 2, \cdots 9$
- Potential for overfitting and lack of identifiability.

Issues

- Model can fit well to data, solutions far from *true* parameter values.
- Can we diagnose such overfitting? Can we mitigated it?
- **Model discrepancy** can reduce the identifiability of the calibration parameters and lead to systematic bias.



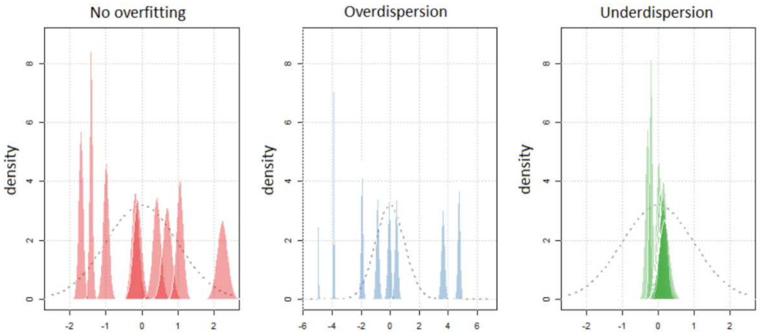
Nuisance parameters and overfitting

- **Aluminum and Tantalum thickness parameters:** These nuisance parameters are measured with a device which we believe to be well registered.
- Measurement error is *exclusive source* of uncertainty. The prior mean and variance of these nuisance parameters are well known.
- Nuisance parameters are standardized (mean 0, variance 1).
- The *standard informative (SI) prior* is:

$$(\gamma_{k1}, \gamma_{k2}, \cdots \gamma_{k9}) \sim N(0, I_9), \; k = 2, 3, 4.$$

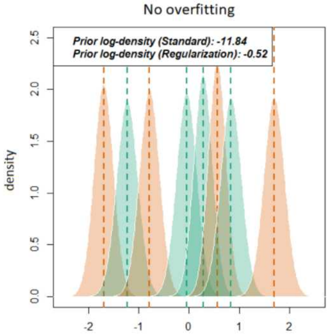
- "True values" are expected to look like a draw from a $N(0, I_9)$ distribution.

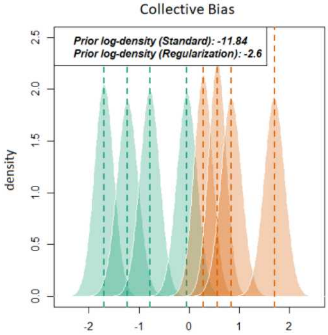
Nuisance parameters and overfitting



- Left panel: agrees with standard prior.
- Middle and left: can lead to overfitting.

Collective Bias for 2 nuisance-sets





- Left: No grouping occurs.
- Right: Collective bias implies systematic overfitting across experiments.
- Standard prior assigns same values.

A metric for overfitting

- We define,

$$M_\gamma = \frac{1}{p}\sum_{j=1}^{p}\gamma_j \qquad V_\gamma = \frac{1}{p-1}\sum_{j=1}^{p}\left(\gamma_j - M_\gamma\right)^2$$

- Prior beliefs about problem structure suggests:

$$M_\gamma \approx 0 \qquad V_\gamma \approx 1$$

- Under standard normal,

$$\pi_{M_\gamma, V_\gamma}(m, v) = N(m \mid 0, 1/p) \times \left[(p-1)\chi^2(v(p-1) \mid p-1)\right]$$

- Reasonable to check that the estimates $\hat{M}_\gamma$ and $\hat{V}_\gamma$ are *coherent* with prior.

A metric for overfitting

- **Definition:** We say that (m, v) is *more coherent with the prior* than (m', v') if

$$\pi_{M_\gamma, V_\gamma}(m, v) > \pi_{M_\gamma, V_\gamma}(m', v')$$

- Define the set of all points which are less coherent with the prior than $(\hat{M}_\gamma, \hat{V}_\gamma)$

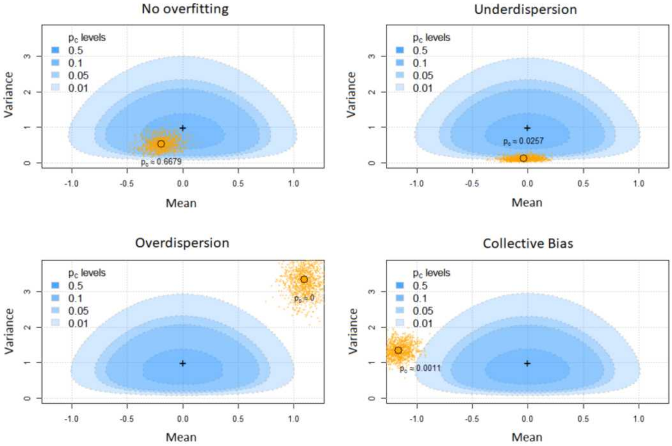
$$\Gamma_{\hat{M}_\gamma, \hat{V}_\gamma} = \left\{ (m, v) \mid \pi_{M_\gamma, V_\gamma}(\hat{M}_\gamma, \hat{V}_\gamma) > \pi_{M_\gamma, V_\gamma}(m, v) \right\}$$

- *Probability of prior coherency* of $(\hat{M}_\gamma, \hat{V}_\gamma)$

$$p_c(\hat{M}_\gamma, \hat{V}_\gamma) = \int_{\Gamma_{\hat{M}_\gamma, \hat{V}_\gamma}} \pi_{M_\gamma, V_\gamma}(m, v) \, dmdv$$

$$\approx \frac{1}{L} \sum_{\ell=1}^{L} \mathbb{1} \left(\pi_{M_\gamma, V_\gamma}(\hat{M}_\gamma, \hat{V}_\gamma) > \pi_{M_\gamma, V_\gamma}(m_\ell, v_\ell) \right)$$

Diagnostic plot for simulated case $p = 10$



- Orange: Point estimates and posterior draws of (M_γ, V_γ)
- Blue: Prior probability contours.

The moment penalization prior

- Overfitting of nuisance parameters leads to $(\hat{M}_\gamma, \hat{V}_\gamma)$ with low prior coherency.
- The *moment penalization (MP) prior* **penalizes** solutions with low prior coherency.
- Using a square loss function,

$$pen_\lambda(\boldsymbol{\gamma}) = \lambda_1(M_\gamma - 0)^2 + \lambda_2(V_\gamma - 1)^2$$

- Prior:

$$\pi_\gamma^{MP}(\boldsymbol{\gamma}) \propto exp\left(-pen_\lambda(\boldsymbol{\gamma})\right)$$

- Tries to encourage solutions with $M_\gamma \approx 0$ and $V_\gamma \approx 1$.

The moment penalization prior

- Therefore,

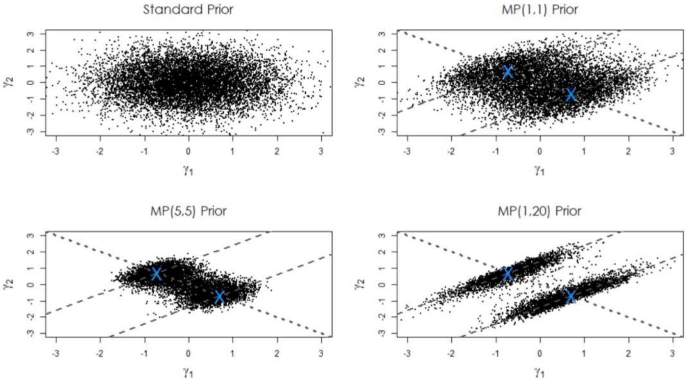
$$\pi_{\gamma}^{MP}(\boldsymbol{\gamma}) \propto \exp\left[-\lambda_1 M_{\gamma}^2\right] \; \exp\left[-\lambda_2 (V_{\gamma} - 1)^2\right]$$

- λ_1 and λ_2 control how strongly we want to enforce constraints.
- *Reparameterize:* $\omega_1 = 2Var(M_{\gamma})\lambda_1$ and $\omega_2 = 2Var(V_{\gamma})\lambda_2$
- Write $\boldsymbol{\gamma} \sim MP(\omega_1, \omega_2)$ to mean that,

$$\pi_{\gamma}^{MP}(\boldsymbol{\gamma}) \propto \exp\left[-\frac{p\omega_1}{2} M_{\gamma}^2\right] \; \exp\left[-\frac{(p-1)\omega_2}{4} (V_{\gamma} - 1)^2\right]$$

- $\boldsymbol{\gamma} \sim MP(1,1)$ is the *standard moment penalization prior.*

Samples from the Standard MP prior



- $10,000$ draws via M-H for $p = 2$.
- As $\omega_1, \omega_2 \to \infty$ all density is placed on $\pm(1/\sqrt{2}, -1/\sqrt{2})$ (Z-regularization).
- As p grows, the induced marginal priors become $N(0,1)$.

Example: The simple machine

- Brynjarsdottir and O'Hagan (2014): The simple machine delivers work

$$\zeta(x) = \frac{E\,x}{1 + x/20}$$

  - x is the amount of *effort* put into the machine.
  - E is the *efficiency* of the machine.
  - Denominator accounts for loss of work due to *friction*.
- The naive simulator introduces model discrepancy

$$\eta(x, E) = Ex$$

Example: The simple machine

- We consider $p = 10$ simple machines, and introduce base efficiency G_j as a machine-dependent nuisance parameter.
- Inputs $x_1, x_2, \cdots x_n$ evenly spaced over $[1, 4]$
- Data generating process:

$$y_{ij} = G_j + \frac{E\, x_i}{1 + x_i/20} + \epsilon_i$$
$$G_j \sim N(0, 0.05^2)$$
$$\epsilon_i \sim N(0, 0.01^2)$$

- Naive simulator:

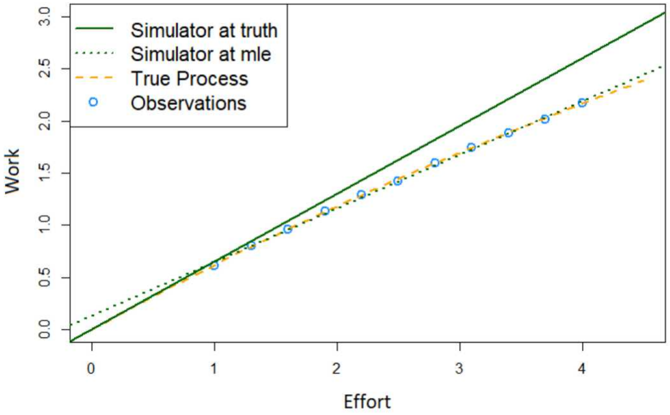
$$\eta(x, E, G) = G + E\, x$$

- True efficiency is $E = 0.65$. Standardize parameters:

$$\alpha = \frac{E - 0.65}{0.3} \sim N(0, 1) \qquad \gamma_k = \frac{G_k - 0}{0.05} \sim N(0, 1)$$

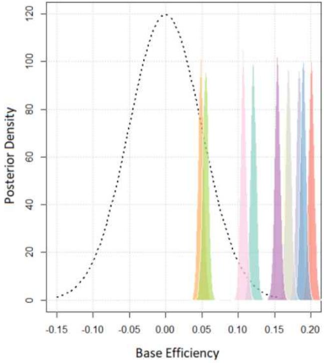
Example: The simple machine

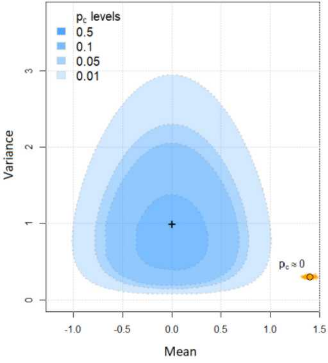
- Model discrepancy leads to *systematic bias.*



Example: The simple machine

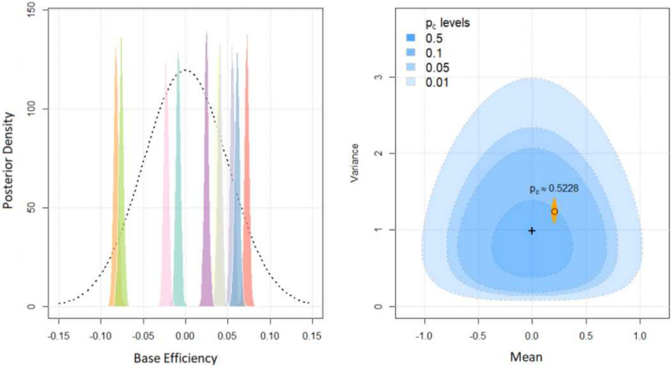
- Under standard informative prior



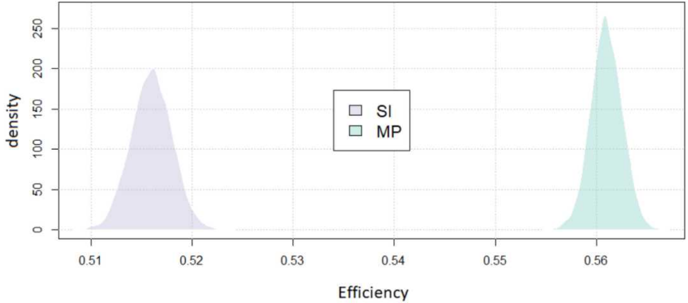


Example: The simple machine

- Under moment penalization prior



Example: The simple machine



- Posterior inference improves under MP, but is still far from truth.
- This is still valuable information! Model discrepancy is leading to biased inference on the parameter of interest.

Dynamic material property calibration revisited

- Inference for two material properties of Tantalum.
- B_0 and B_0' are the Bulk modulus of tantalum and its pressure derivative.

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2) = (B_0, B_0')$$

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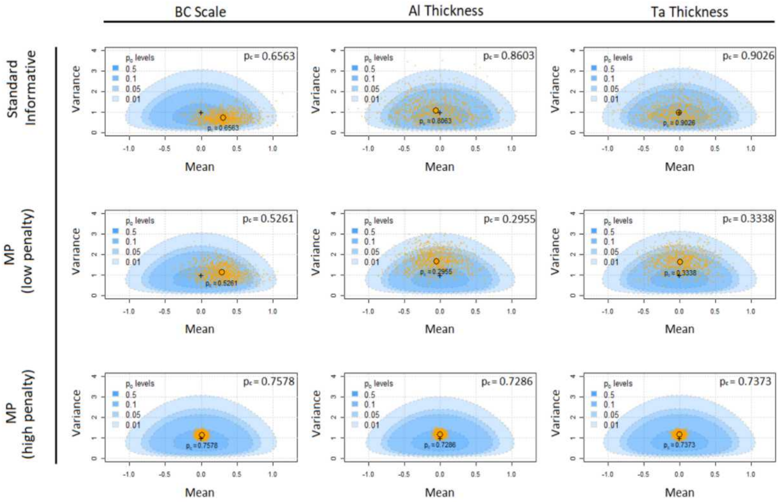
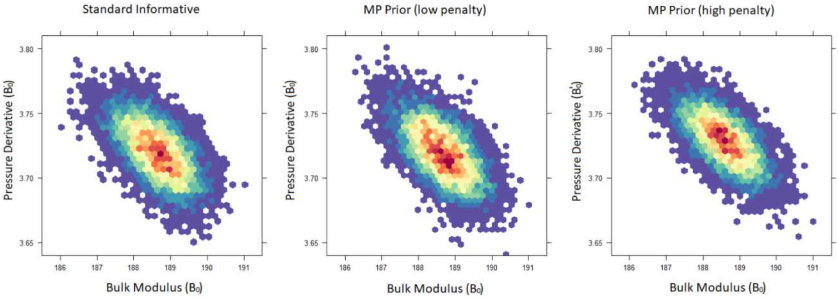
- Perform BMC for SI, SMP and MP(20, 40) priors.

Dynamic material property calibration
Diagnostic plots



Dynamic material property calibration Physical parameter posteriors



- Similar posterior inference in all cases.
- Indicates that model discrepancy is unlikely to be causing bias in the parameters of interest.

Conclusions

- Overfitting of nuisance parameters leads to systematic bias which is often a symptom of model discrepancy.
- In complex high-dimensional problems, with appropriate problem structure, we can:
    - **Identify:** Probability of prior coherency identifies many types of overfitting, should it occur.
    - **Reduce:** The moment penalization prior reduces the systematic bias of the nuisance parameters.
    - **Diagnose:** Examine the sensitivity of posterior inference in order to diagnose the presence and effect of model discrepancy on the parameters of interest.

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