Laboratories

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"Learn something new: techniques for broadening your statistical skillset."

PRESENTED BY

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Dr. Minnier's: "Sharpening..."

- Statistics is shifting and we need to "sharp" our skill.
- We all have something new to learn.
- R is more "fun" and not "slow"
- As reference, back in the mid 90?s
  - Unix workstations
  - We had "Splus?
  - Programming in Fortran and C.
  - No tidy verse, etc.
- Lots to learn and practical advise.
- "Practice" and "move out of your comfort zone".

Dr. Mannhardt's: "Flipping..."

- Let us be research partners in the collaborative work.
- How to best communicate statistical findings to non-statisticians?
- When communicating with decision leaders and non-statistics experts lets emphasize:
  - Our bottom line.
  - Acknowledge communication styles.
  - Team work. ("I" in Statistics but not in Team).
  - How are we teaching our students?
- Message: Our methods/computations/technical skill are important but managers don?t want to learn or know all the details.
  - What are the implications of an analysis?
  - How does this support answers to decision maker questions or problems?

Dr. Calder's "Feasibility and Validity..."

- Analysis of complex data for adolescence development: survey + GPS data.
- Large effort to assess noise of GPS data (space-time budget).
- *Multilevel Negative Binomial:* Number of missing minutes of GPS coverage.
- *Multilevel Logistic Regresion:* Discordance of GPS and "space-time budget",
- Effects studied thru a range of models with interpretable results.
- Models build with an increasing number of covariables.

Dr. Wenderlberger's. "Thinking..."

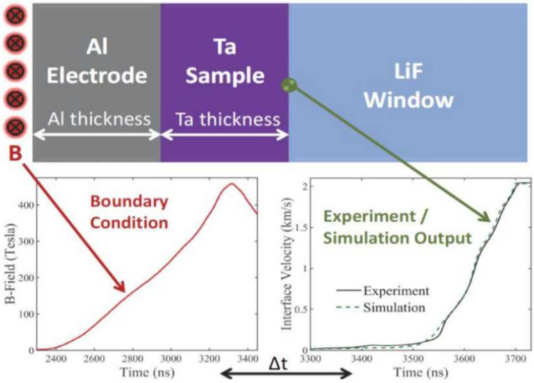
- Illustrates "diverse skill set" around problems at LANL.
- Highlights research process and collaboration.
- Stating problem; $\rightarrow$ Data; $\rightarrow$; useful methods/techniques
- Functional data for "Uncertainty Quantification".
    - Given a series of inputs/outputs, from high scale computer simulations,
    - How do we best represent the input/functional output relationship without running the computer code?
    - Build a "surrogate" or "emulator".
    - Duality to multivariate statistics.

Calibration in material sciences [1]

- **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.

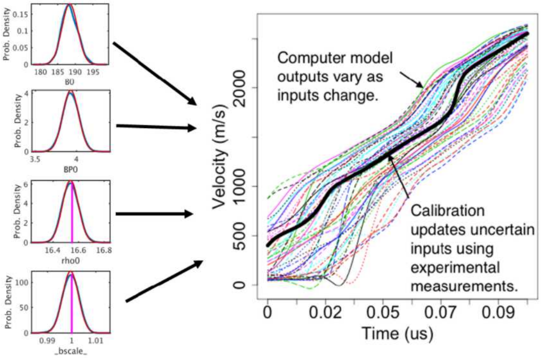
[1] work with Kellin Rumsey, Lauren Hund and Derek Tucker (SNL)

Experimental setup



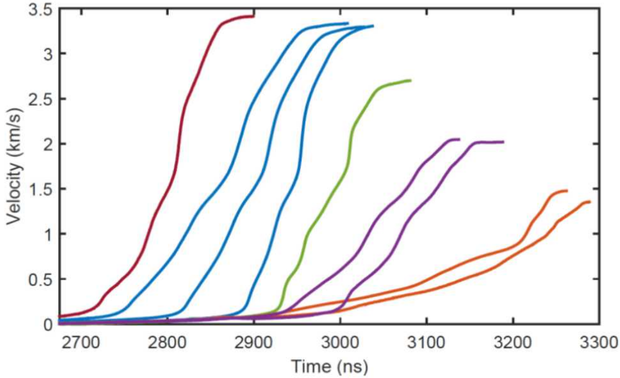
- "By coupling experimental and simulated velocity traces, parameters of the tantalum (Ta) equation of state (EOS) can be estimated".
- Massive electric currents treated as boundary conditions.

Calibration



- Uncertain inputs generate velocity curves using a computer model.
- Probability distributions look for ”agreement” of outputs and measurements.

Challenges



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

Framework

- Following Kennedy & O'Hagan 2001, model the i^{th} observation in the j^{th} experiment as,

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

- $\boldsymbol{\alpha}$ 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

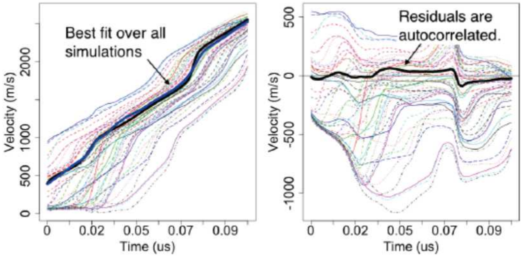
- BMC framework to obtain inference for two material properties of Tantalum.
- B_0 and B_0' are the Bulk modulus of tantalum and its pressure derivative.

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

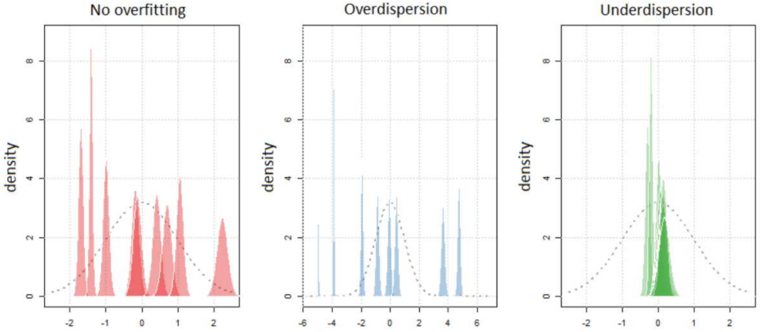
- Four nuisance that may vary across $p = 9$ experiments
  - Tantalum density - γ_1
  - Magnetic field scaling - γ_{2j}, $j = 1, 2, \cdots 9$
  - Aluminum thickness- γ_{3j}, $j = 1, 2, \cdots 9$
  - Tantalum thickness - γ_{4j}, $j = 1, 2, \cdots 9$
- Potential for overfitting and lack of identifiability.

Issues

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

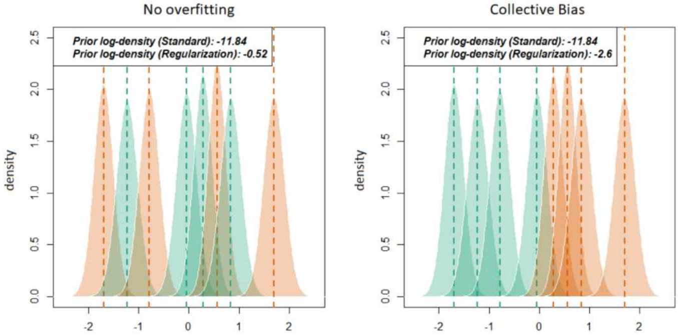


Nuisance parameters and overfitting



- Left panel: agrees with standard prior.
- Middle and left: situation that 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.

The MP prior

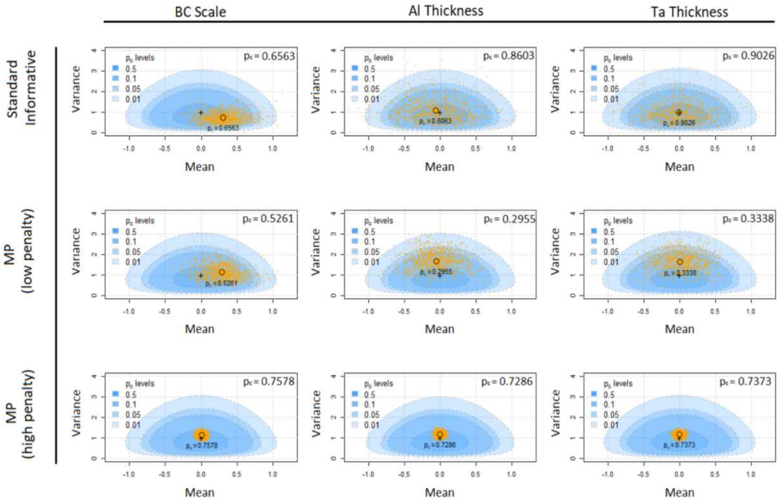
- The *moment penalization (MP) prior* **penalizes** solutions with *low prior coherency*.
- Let $h_a(x)$ be a function which takes larger values when x is close to a.

$$\pi_{\gamma}^{MP}(\boldsymbol{\gamma}) \propto h_0(M_\gamma) h_1(V_\gamma)$$

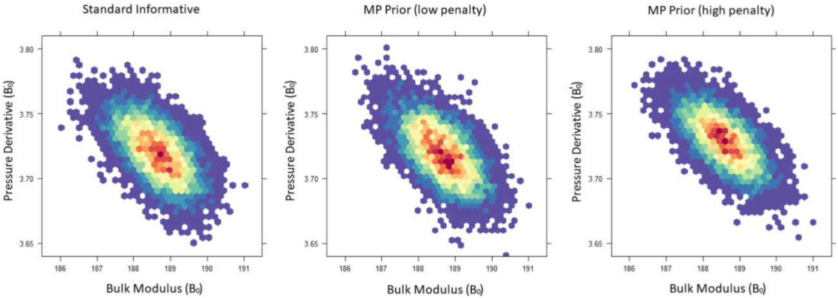
- Tries to encourage solutions with

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

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.