Two Approaches to Calibration in Metrology

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Abstract: Inferring mathematical relationships with quantified uncertainty from measurement data is common to computational science and metrology. Sufficient knowledge of measurement process noise enables Bayesian inference. Otherwise, an alternative approach is required, here termed *compartmentalized inference*, because collection of uncertain data and model inference occur independently. Bayesian parameterized model inference is compared to a Bayesian-compatible compartmentalized approach for ISO-GUM compliant calibration problems in renewable energy metrology. In either approach, model evidence can help reduce model discrepancy.

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Outline

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1. The Problem of Calibration in Metrology
2. 1st Approach: Bayesian Inference
3. 2nd Approach: Compartmentalized Inference
4. Summary

The Measurement Problem

A **measuring system** can be represented by the statistical model

$$y = g(x; \boldsymbol{\theta}) + \varepsilon,$$

where we seek to measure the **quantity value** x, and

- the **indication** y is generated by the measuring system,
- ε is the noise in the indication, with a distribution model,
- the function g models the measuring system, and
- the **calibration parameter** θ parameterizes g.

The measuring system transforms the **unobservable** x into the **observable** y.

Sources of Uncertainty I

Example (Affine Measuring System):

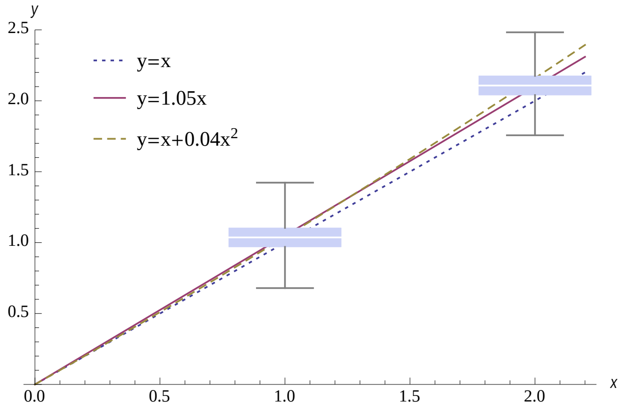
$$y = g(x; \boldsymbol{\theta} = (a_0, a_1)^{\mathsf{T}}) + \varepsilon = \overbrace{a_0}^{\text{offset}} + \overbrace{a_1}^{\text{gain}} x + \varepsilon, \quad \varepsilon \sim \mathcal{N}\left(0, \sigma_\varepsilon^2\right).$$

If the measuring system can be "zeroed" (e.g., a mass scale), then we have a Linear Measuring System with $a_0 = 0$.

Major sources of uncertainty in x from observation y:

1. Noise ε in the indication.
2. Calibration uncertainty in the parameter $\boldsymbol{\theta}$, potentially including instrument drift.
3. Inadequacy of the model for ε, e.g., distribution type, independence, heteroscedasticity, uncertainty in σ_ε^2.
4. Inadequacy of the model g, or model error/discrepancy.

Sources of Uncertainty II



Zero a scale, then determine gain using two reference weights.

Reference uncertainty in x combined with indication noise in y.

Bayesian Inference vs. "Forward" Unc. Propagation I

Example (Linear Measuring System):

$$y = g(x; a_1) + \varepsilon = a_1\, x + \varepsilon, \quad \varepsilon \sim \mathcal{N}\left(0, \sigma_\varepsilon^2\right), \quad \sigma_\varepsilon^2 \text{ is known.}$$

Bayesian Measurement Inference: Via Bayes' theorem, the likelihood function L transforms a prior **state-of-knowledge distribution** (SoKD) for X and A_1 into a posterior SoKD for X and A_1. (Finite indication resolution assumed negligible.)

$$Y|X = x, A_1 = a_1 \sim \mathcal{N}(\overbrace{a_1\, x}^{g(x;\, a_1)}, \sigma_\varepsilon^2), \quad \text{(observation distribution)}$$

whose probability density function (PDF) defines L:

$$f_{Y|X,A_1}(y|X = x, A_1 = a_1) = \frac{e^{-\frac{(y - a_1\, x)^2}{2\,\sigma_\varepsilon^2}}}{\sqrt{2\,\pi}\,\sigma_\varepsilon} =: L(x, a_1; y).$$

Bayesian Inference vs. "Forward" Unc. Propagation II

Bayes' theorem for (joint) inference of X and A_1:

$$f^{\text{post}}_{X,A_1|Y}(x, a_1 | Y = y) = \frac{L(x, a_1; y) \overbrace{f^{\text{prior}}_X(x)\, f^{\text{prior}}_{A_1}(a_1)}^{\text{independent priors}}}{\underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} L(\xi, \alpha_1; y) f^{\text{prior}}_X(\xi) f^{\text{prior}}_{A_1}(\alpha_1) \mathrm{d}\xi\, \mathrm{d}\alpha_1}_{\text{evidence for } g \text{ is usually hard to compute}}}$$

Typically, X's prior is "diffuse", and A_1's prior is "sharp", and much more information is gained about X than A_1.

Integrate out A_1 to get the marginal posterior for X.

μ_X and σ_X summarize the measurement, according to the *Guide to the Expression of Uncertainty in Measurement (GUM)*.

Bayesian Inference vs. "Forward" Unc. Propagation III

Psuedo-inversion: In practice, the Measurement Problem is often "inverted" in a somewhat ad hoc manner.

The noise ε is used to derive first a SoKD for Y (GUM Type A), and then g is inverted to give a **measurement function** to propagate uncertainty, giving X's SoKD:

$$X = C\,Y, \quad \text{(e.g., "forward" MC sampling computes } X\text{)}$$

where the prior for A_1 is replaced by a SoKD for C (Type B).

Roughly speaking, $C \approx 1/A_1$.

Among other issues, g may be impossible/impractical to invert.

The Calibration Problem I

Example (Linear Measuring System):

$$y = g(x; a_1) + \varepsilon = a_1\, x + \varepsilon, \quad \varepsilon \sim \mathcal{N}\left(0, \sigma_\varepsilon^2\right), \quad \sigma_\varepsilon^2 \text{ is known.}$$

Recall: The "sharp" prior for the calibration parameter A_1 enabled strong inference about a "diffuse" X prior.

Calibration reverses these roles.

A "sharp" prior for X enables strong inference about a "diffuse" A_1 prior.

"Sharp" priors for X are provided by **measurement standards** (a.k.a. **references**) with the SoKD summarized in a **calibration certificate**.

The Calibration Problem II

Bayesian Calibration Inference:

$$f^{\text{post}}_{X,A_1|Y}(x, a_1|Y = y) = \frac{L(x, a_1; y) f^{\text{prior}}_X(x)\, f^{\text{prior}}_{A_1}(a_1)}{\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} L(\xi, \alpha_1; y) f^{\text{prior}}_X(\xi) f^{\text{prior}}_{A_1}(\alpha_1) \mathrm{d}\xi\, \mathrm{d}\alpha_1}$$

Typically, A_1's prior is "diffuse", and X's prior is "sharp", and much more information is gained about A_1 than X.

Integrate out X to get the marginal posterior for A_1.

Calibration may involve multiple references, $X_1, \ldots, X_N$, which may not be independent.

Certain References, Known Noise in Indications

Sometimes, references have negligible uncertainty, and ≥ 1 indications are taken for each reference $x_1, \ldots, x_M$, giving a vector $\boldsymbol{y}$ of $N \geq M$ indications.

For the Linear Measuring System with an improper, uniform prior on A_1, this gives Bayesian linear regression for A_1, where

$$A_1 \sim \mathcal{N}\left(\mu_{A_1}, \sigma^2_{A_1}\right), \text{ with}$$

$$\mu_{A_1} = (\mathcal{X}^\mathsf{T}\mathcal{X})^{-1}\mathcal{X}^\mathsf{T}\boldsymbol{y} \quad \text{and} \quad \sigma^2_{A_1} = (\mathcal{X}^\mathsf{T}\mathcal{X})^{-1}\sigma^2_\varepsilon,$$

and where $\mathcal{X} := \underbrace{(x_1, \ldots, x_M)}_{\text{length } N}{}^\mathsf{T}$ is the design matrix.

Evidence for different g choices can be readily computed!

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1st Approach: Bayesian Inference

In general, references $(X_1, \ldots, X_M) =: \boldsymbol{X}$ have non-negligible uncertainty. Their priors are updated along with the calibration parameter A_1.

One independent indication from each of two independent references gives

$$\begin{aligned} f^{\text{post}}_{\boldsymbol{X},A_1|\boldsymbol{Y}}(\boldsymbol{x}, a_1 | \boldsymbol{Y} = \boldsymbol{y}) &\propto L(\boldsymbol{x}, a_1; \boldsymbol{y}) f^{\text{prior}}_{\boldsymbol{X}}(\boldsymbol{x})\, f^{\text{prior}}_{A_1}(a_1) \\ &= f_{Y_1}(a_1\, x_1)\, f_{Y_2}(a_1\, x_2)\, f_{X_1}(x_1)\, f_{X_2}(x_2). \end{aligned}$$

where

$$Y_1 \sim \mathcal{N}\left(y_1, \sigma_\varepsilon^2\right) \quad \text{and} \quad Y_2 \sim \mathcal{N}\left(y_2, \sigma_\varepsilon^2\right).$$

Marginalizing out the references gives

$$f_{A_1}(a) \propto \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{Y_1}(a_1\, x_1)\, f_{Y_2}(a_1\, x_2)\, f_{X_1}(x_1)\, f_{X_2}(x_2)\, \mathrm{d}x_1 \mathrm{d}x_2.$$

Example: Bayesian Inference I

True values:

$$x_1^{\text{true}} = 0.997 \qquad y_1^{\text{ind}} = 1.037 \qquad a_1^{\text{true}} = 1.05$$

$$x_2^{\text{true}} = 1.998 \qquad y_2^{\text{ind}} = 2.108 \qquad \sigma_\varepsilon = 0.01$$

Prior Knowledge:

$$X_1^{\text{prior}} \sim \mathcal{U}(0.99, 1.01)\,, \qquad \frac{\sigma_{X_1^{\text{prior}}}}{|\mu_{X_1^{\text{prior}}}|} = 0.577\%, \qquad f_{A_1}^{\text{prior}}(a_1) \propto 1,$$

$$X_2^{\text{prior}} \sim \mathcal{U}(1.99, 2.01)\,, \qquad \frac{\sigma_{X_2^{\text{prior}}}}{|\mu_{X_2^{\text{prior}}}|} = 0.289\%,$$

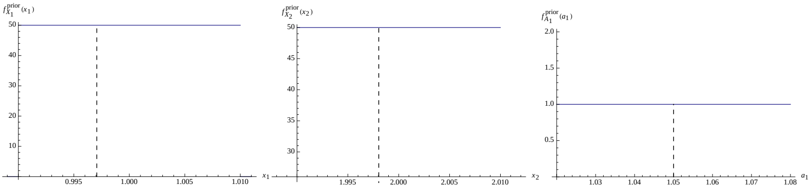
Posterior Knowledge Summary:

$$\mu_{X_1^{\text{post}}} = 0.997 \qquad \frac{\sigma_{X_1^{\text{post}}}}{|\mu_{X_1^{\text{post}}}|} = 0.381\% \qquad \mu_{A_1^{\text{post}}} = 1.048$$

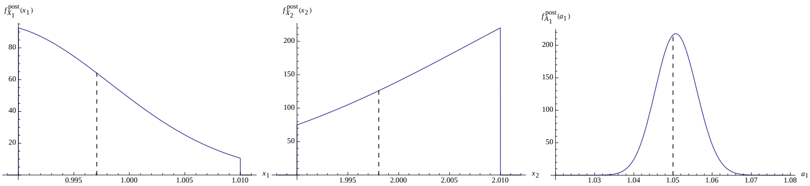
$$\mu_{X_2^{\text{post}}} = 2.008 \qquad \frac{\sigma_{X_2^{\text{post}}}}{|\mu_{X_2^{\text{post}}}|} = 0.050\% \qquad \frac{\sigma_{A_1^{\text{post}}}}{|\mu_{A_1^{\text{post}}}|} = 0.441\%$$

Example: Bayesian Inference II

Priors:



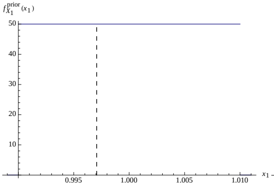
Posteriors (quadrature using Mathematica's `Integrate`):

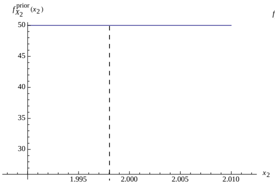


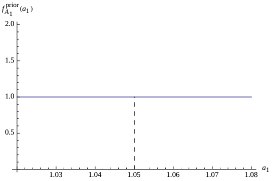
X_1 X_2 A_1

Example: Bayesian Inference III

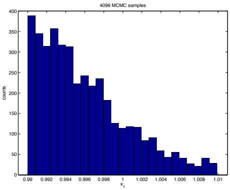
Priors:



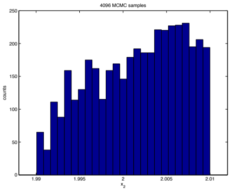




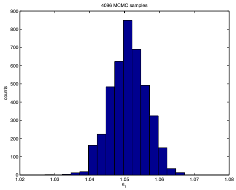
Posteriors (MCMC using MATLAB's `mhsample`):



X_1



X_2



A_1

Outline

2^{nd} Approach: Compartmentalized Inference

For some measurement processes it may be that

- parameter inference occurs separately from data collection, and/or
- an indication Y may be given as a SoKD without any associated noise model (e.g., from instrument spec's).

In addition, how might one motivate Bayesian calibration to an engineer/technician by using, say, a more intuitive idea of "forward" propagation of distributions?

We will handle such **compartmentalized inference** in Bayesian-compatible way, and create a SoKD for A_1.

Compartmentalized Inference: Derivation I

Motivation:
Start with the CDF for Y using the Heaviside function:

$$F_Y(y) = \int_{-\infty}^{\infty} H(y - a_1\, x)\, f_{A_1,X}(a_1, x)\, \mathrm{d}a_1\, \mathrm{d}x$$

Differentiate w.r.t. y using the δ function to give the PDF:

$$f_Y(y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(y - a_1\, x)\, f_{A_1,X}(a_1, x)\, \mathrm{d}a_1\, \mathrm{d}x$$

Can sample from $Y's$ distribution using forward MC:

$$\mathrm{E}(Y) = \int_{-\infty}^{\infty} y\, f_Y(y)\, \mathrm{d}y = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} a_1\, x\, f_{A_1,X}(a_1, x)\, \mathrm{d}a_1\, \mathrm{d}x$$

Compartmentalized Inference: Derivation II

Change perspective to A_1 from Y (rigorous δ "sifting"?!?):

$$f_{A_1}(a) \overset{!!!}{\propto} \iiiint_{-\infty}^{\infty} \delta(y_1 - a_1\, x_1)\,\delta(y_2 - a_1\, x_2)\; f_{X_1}(x_1)\, f_{Y_1}(y_1)\, f_{X_2}(x_2)\, f_{Y_2}(y_2)\, \mathrm{d}x_1 \mathrm{d}y_1 \mathrm{d}x_2 \mathrm{d}y_2$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{X_1}(x_1)\, f_{Y_1}(a_1\, x_1)\, f_{X_2}(x_2)\, f_{Y_2}(a_2\, x_2)\, \mathrm{d}x_1 \mathrm{d}x_2$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{Y_1}(a_1\, x_1)\, f_{Y_2}(a_2\, x_2)\, f_{X_1}(x_1)\, f_{X_2}(x_2)\, \mathrm{d}x_1 \mathrm{d}x_2$$

This is the **same** as the marginal posterior PDF for A_1 from the Bayesian analysis, up to normalization!

Outline

Summary and Areas to Explore

- A Bayesian approach unifies the Measurement Problem with the Calibration Problem, without ad hoc inversion.
- The Compartmentalized approach ended up being equivalent to a particular Bayesian inference.

- When are the two approaches equivalent?
  (For example, add unknown variance in indications.)
- Can/should model selection be based upon minimal posterior uncertainty instead of evidence?
- Standard methods and automated computational tools?
  (As easy as Excel's linear fit with an R^2 metric?!?)

Questions?

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