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Bayesian Information Fusion for Model Calibration, Validation, and Prediction

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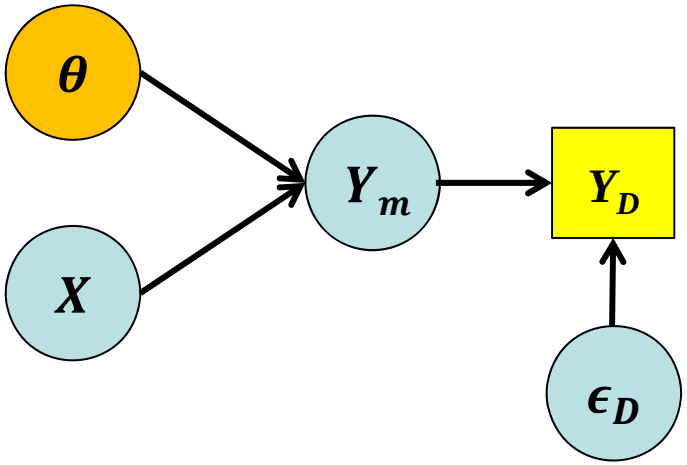
Outline

1. Model calibration
2. Model validation
3. Integration of calibration and validation results
4. Prediction

1. Bayesian Calibration → Case 1

- $\boldsymbol{\theta}$ is an unknown constant
- Likelihood function based only on measurement error ($\boldsymbol{X}$ and $\boldsymbol{Y}$)
  - $Y_D(\boldsymbol{X}) = Y_m(\boldsymbol{X}, \boldsymbol{\theta}) + \varepsilon_D$
  - $\varepsilon_D \sim N(0, \sigma_D)$
- Update distribution of $\boldsymbol{\theta}$ with data



$$f(\boldsymbol{\theta}|Y_D) = \frac{\Pr(Y_D|\boldsymbol{\theta}) f(\boldsymbol{\theta})}{\int \Pr(Y_D|\boldsymbol{\theta}) f(\boldsymbol{\theta}) d\boldsymbol{\theta}}$$

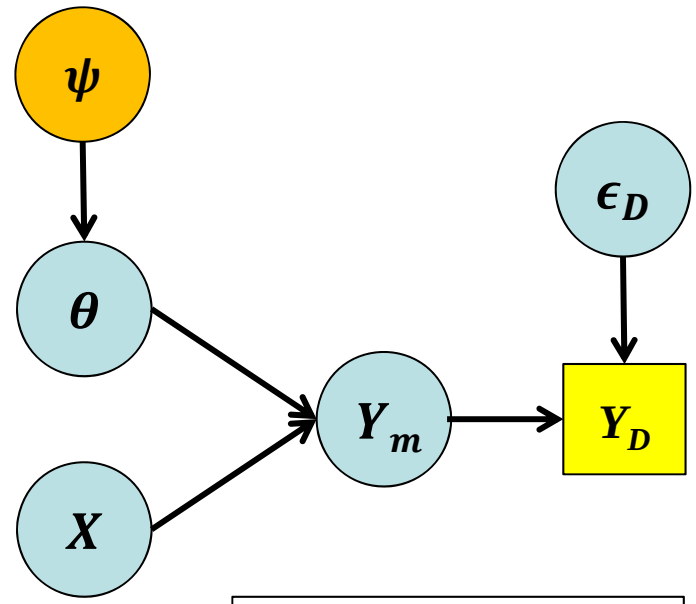
$\boldsymbol{X} \rightarrow \{P, \chi, H, x, \phi\}$
$\boldsymbol{Y} \rightarrow \{w, \sigma\}$
$\boldsymbol{\theta} \rightarrow \{E, \nu, T, L, R\}$

Additional observations tend to reduce uncertainty in θ (i.e., distribution converges towards a single value)

Bayesian Calibration → Case 2

- $\boldsymbol{\theta}$ is an unknown random variable
  - $\theta_i \sim f_{\theta_i}(\theta_i | \boldsymbol{\psi_i})$
  - Tank-to-tank variability
- Likelihood based on measurement error ($\boldsymbol{X}$ and $\boldsymbol{Y}$), and variability of $\boldsymbol{\theta}$
  - $Y_D(\boldsymbol{X}) = Y_m(\boldsymbol{X}, \boldsymbol{\theta}) + \varepsilon_D$
  - $\varepsilon_D \sim N(0, \sigma_D)$
- Update distribution of $\boldsymbol{\psi}$ with data

$$f(\boldsymbol{\psi}|Y_D) = \frac{\Pr(Y_D|\boldsymbol{\psi}) f(\boldsymbol{\psi})}{\int \Pr(Y_D|\boldsymbol{\psi}) f(\boldsymbol{\psi}) d\boldsymbol{\psi}}$$



$\boldsymbol{X}$ → $\{P, \chi, H, x, \phi\}$
$\boldsymbol{Y}$ → $\{w, \sigma\}$
$\boldsymbol{\theta}$ → $\{E, \nu, T, L, R\}$
$\boldsymbol{\psi_i}$ → ????

Additional observations tend to reduce uncertainty in ψ
(i.e., family of distributions of θ converges towards a single distribution)

Johnson family of distributions

PDF: $$f_x(x) = \frac{\delta}{\lambda\sqrt{2\pi}} g'\left(\frac{x-\xi}{\lambda}\right) \exp\left\{-\frac{1}{2}\left[\gamma + \delta \cdot g\left(\frac{x-\xi}{\lambda}\right)\right]^2\right\}$$

CDF: $$F(x) = \Phi\{\gamma + \delta . g[(x-\xi)/\lambda]\}$$

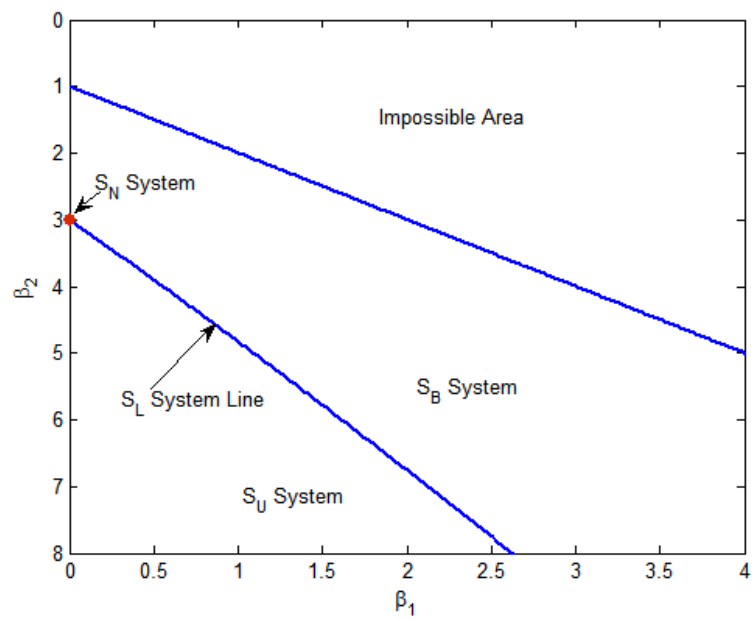
$\boldsymbol{\theta} \rightarrow \{E, \nu, T, L, R\}$

$\boldsymbol{\psi_i} \rightarrow \{\delta_i, \xi_i, \lambda_i, \gamma_i\}$

Inverse CDF: $$Z = \gamma + \delta . g[(x-\xi)/\lambda]$$

Z - standard normal variate

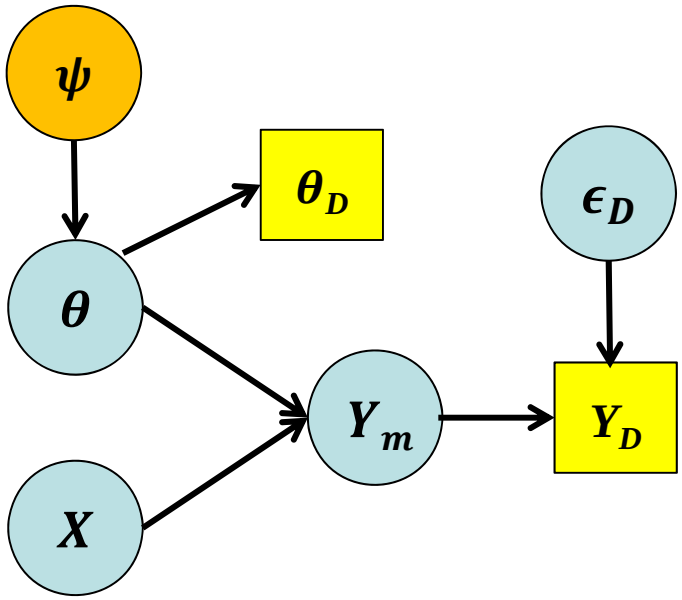
$$g(y) = \ln(y), \text{ for lognormal } (S_L)$$
$$= \ln\left[y + \sqrt{y^2+1}\right], \text{ for unbounded } (S_U)$$
$$= \ln[y/(1-y)], \text{ for bounded } (S_B)$$
$$= y, \text{ for normal } (S_N)$$



$$\beta_1 \equiv m_3^2 / m_2^3 \qquad \beta_2 \equiv m_4 / m_2^2$$

Sequence of two calibrations

- Family of Johnsons for each parameter θ fitted to data sets 2 and 4 (direct measurements) → Bayesian
- This becomes the prior for calibration with data set 5 (measure displacement, no liquid)
- Integrate over distribution parameters ψ to produce unconditional PDF for each θ, for propagation



- Spatial variability within each tank
  - θ is a random field
  - Ergodicity assumption

Gaussian Process (GP) Surrogate Model

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- Calibration with data set 5 is expensive due to the need for nested sampling over aleatory uncertainty (i.e., variability of $\boldsymbol{\theta}$)
  - Surrogate model is necessary even for a relatively cheap model
- GP composed of two parts:
  - Mean function *m* (simple constant used here)
  - Covariance function *k* (squared exponential decay used here)

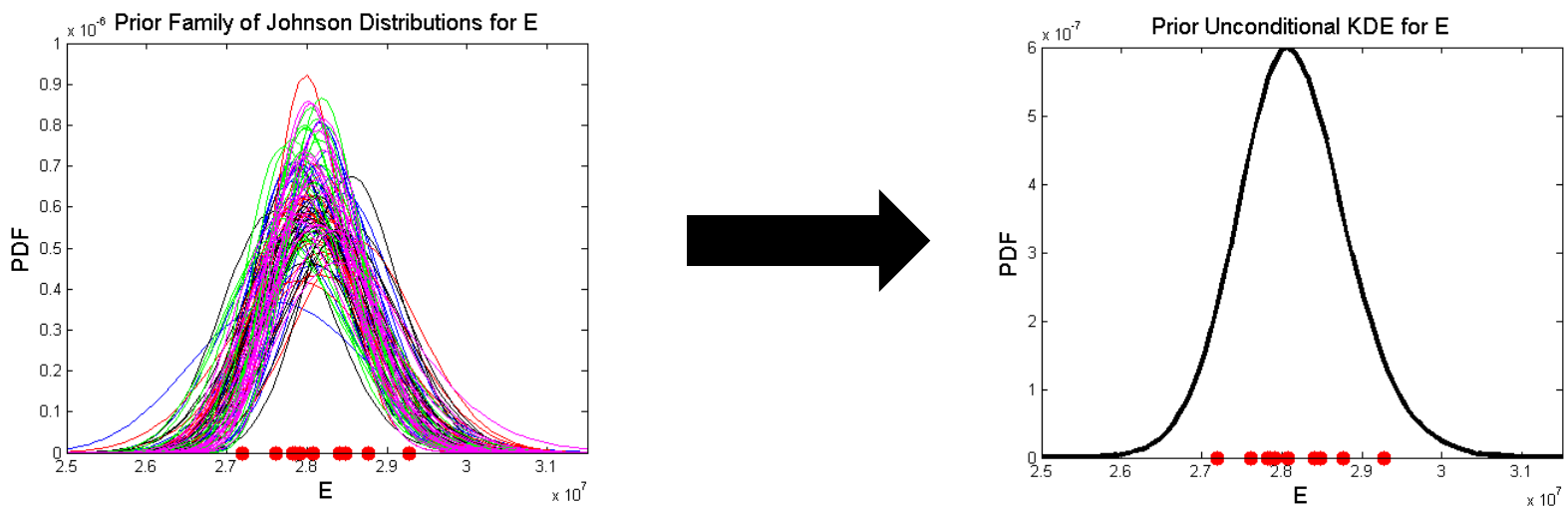
$$k(x_i, x_j) = \gamma \exp\left[-\frac{1}{2}\sum_{d=1}^{D}\frac{(x_i - x_j)^2}{l_d}\right]$$

- GP prediction $\pi(y_P|x_P) \sim N(\mu, \Sigma)$

$$\mu = m(x_P) + K_{PT}(K_{TT} + {\sigma_n}^2 I)^{-1}[y_T - m(x_T)]$$
$$\Sigma = K_{PP} - K_{PT}(K_{TT} + {\sigma_n}^2 I)^{-1} K_{TP}$$

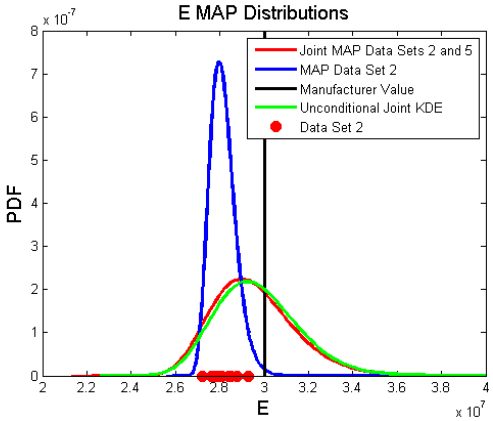
Unconditional distribution

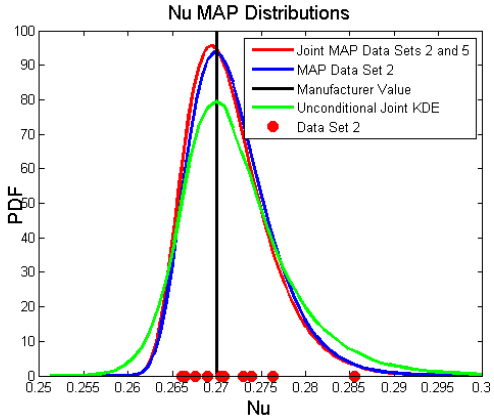
- Integrate over distribution parameters ψ to produce unconditional PDF for each θ, for propagation

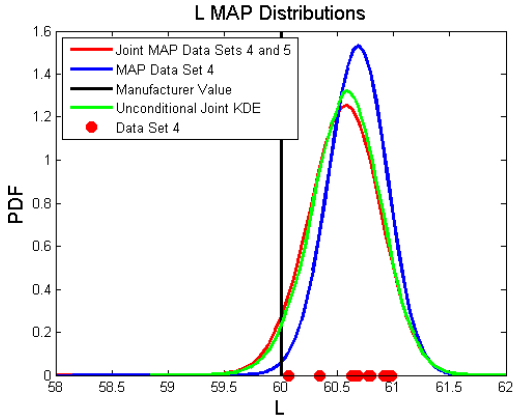


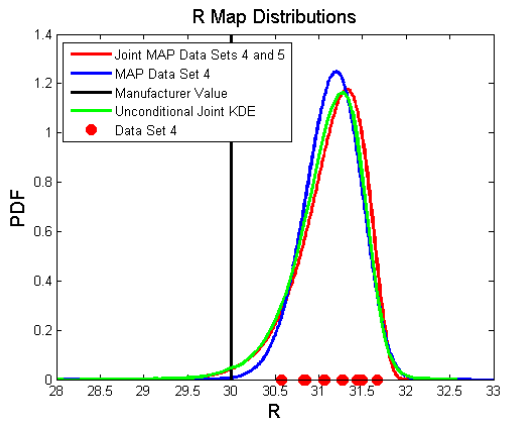
- After integration, the aleatory and epistemic uncertainties can no longer be separated in propagation
- However, need to validate model before propagation

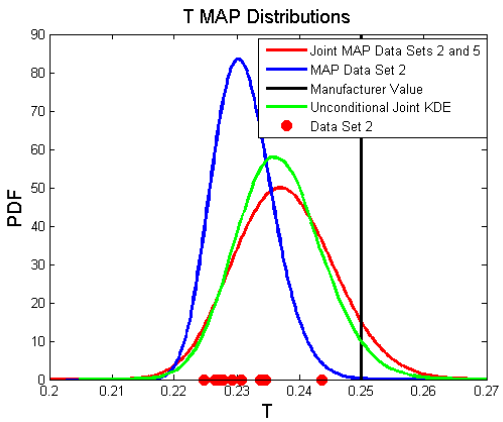
Calibrated Posterior Distributions











2. Model validation

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Quantitative Methods

1. Classical hypothesis testing
2. Bayesian hypothesis testing (equality and interval)
3. Model reliability metric
4. Area metric
5. K-L divergence
6 Real-space comparison

Probability measures → Useful in Roll-up to prediction UQ

Bayesian hypothesis testing

- Comparison of two hypotheses (H_0 and H_1)
  - H_0: model is correct, H_1 : model is incorrect
- Validation metric → Bayes factor

$$B = \frac{\Pr(D \mid H_0)}{\Pr(D \mid H_1)}$$

D → obs data

Prob(model is correct): $\Pr(H_0|D) = B / B+1$

Model reliability metric

- Pred → y Obs → z
- H_0 → $|y - z| \leq \delta$
- Compute $P(H_0)$
- $P(H_1) = 1 - P(H_0)$

Rebba et al, RESS 2006;
Jiang & Mahadevan, RESS 2006;
Rebba & Mahadevan, RESS 2008
Ling & Mahadevan, RESS 2013.

Model Reliability Metric

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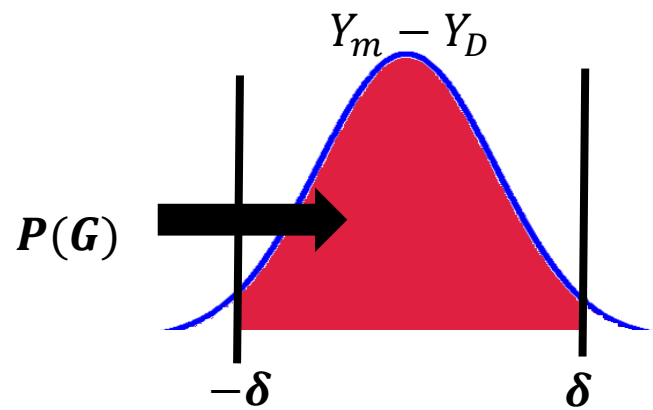
Model reliability metric

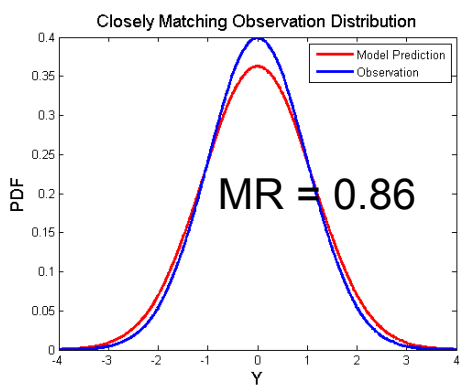
$$P(G) = P(|\boldsymbol{Y_m}(\boldsymbol{X}) - \boldsymbol{Y_D}(\boldsymbol{X})| < \delta)$$

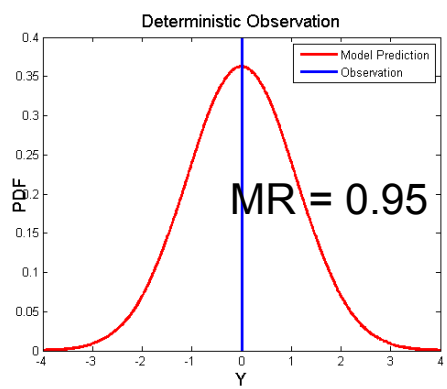
Model prediction affected by

- Epistemic uncertainty about model parameters $\boldsymbol{\theta}$
- Model errors (numerical & model form)



Validation should only assess epistemic uncertainty in model





Reasonable when there is only measurement noise → Spreads in prediction and observation come from different sources

Model Reliability Metric Computation (under aleatory and epistemic uncertainty)

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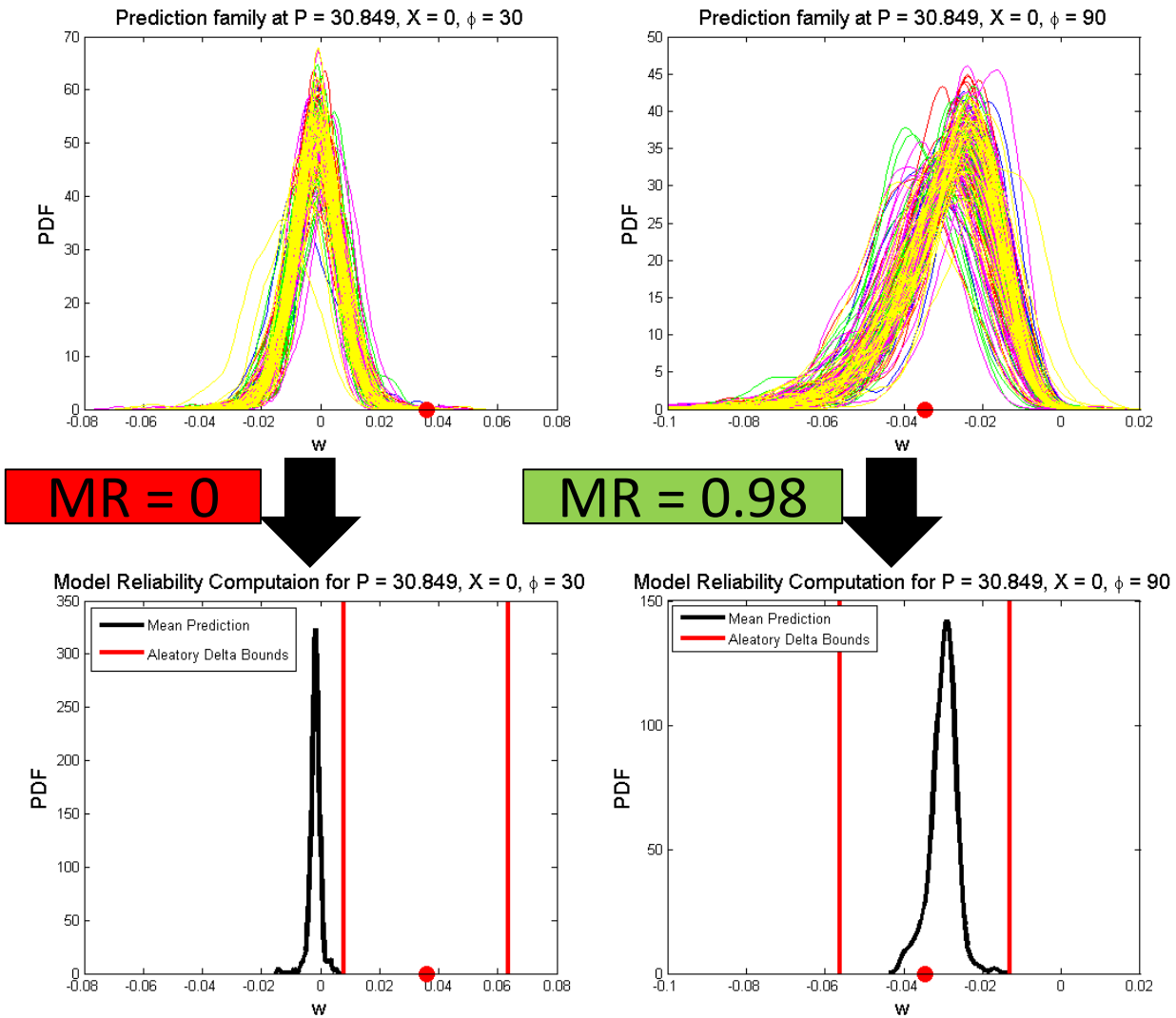
- In the presence of aleatory uncertainty in $\boldsymbol{\theta}$:
  - Integrate prediction over aleatory uncertainty (otherwise will be penalized for aleatory component)
  - $P(G) = P(|E_\theta[\boldsymbol{Y_m}(\boldsymbol{X}, \boldsymbol{\theta})] - \boldsymbol{Y_D}(\boldsymbol{X})| < \delta)$
  - Set the tolerance based on average aleatory uncertainty $E_\psi\left[\sigma_{Y_m}\right]$

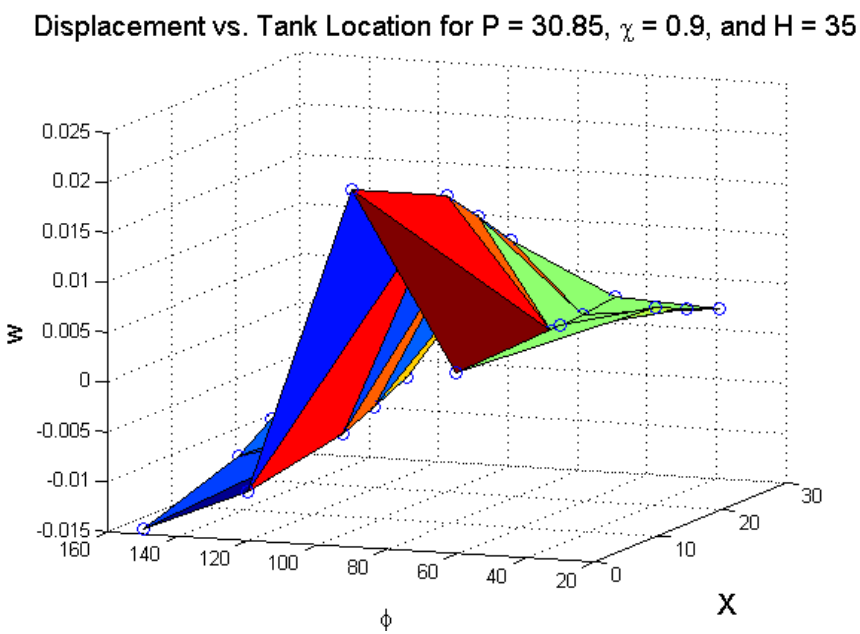
Model Reliability Metric Computation



- Integrate prediction over the aleatory uncertainty
- Mean prediction is then purely epistemic
- Tolerance → Observation $\pm 2\sigma_{Y_m}$
- Tolerance approach is conservative

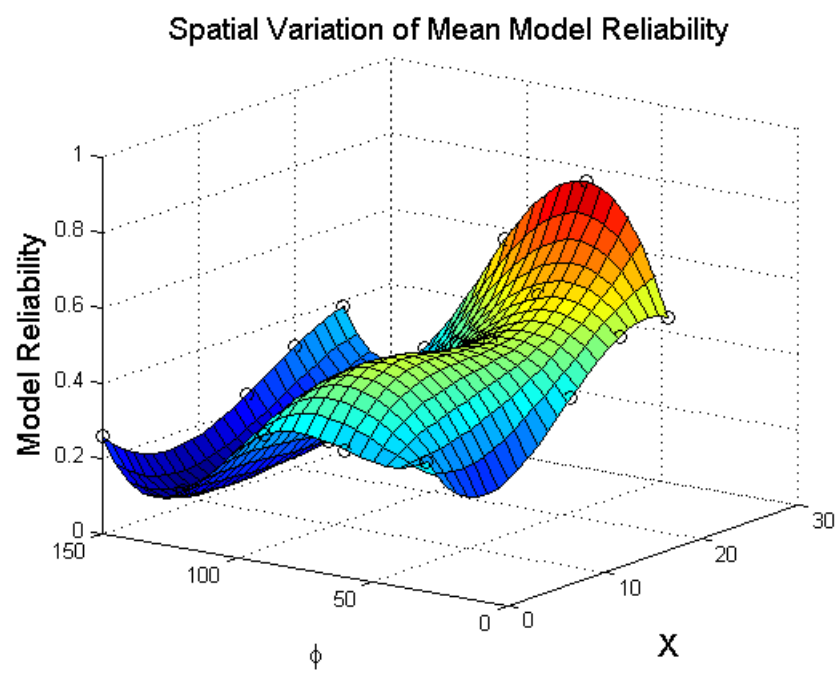
Computational Challenge

- Separation of aleatory and epistemic uncertainty in validation requires a double-loop approach (expensive)
- Two options:
  - Use a surrogate (e.g. GP) and include surrogate error in metric
  - Use original model for sparse sampling and/or parallelize computations
- Displacement response is non-linear across space → need adaptive training point selection



Validation Results

- Mean model reliability at each spatial tank location
  - Averaged over 12 conditions
  - 4 tanks, 3 input conditions
- Model tends to perform better for larger values of X and ϕ
- Mean MR = 0.39 across all 20 inputs and locations



3. Integration of Calibration and Validation

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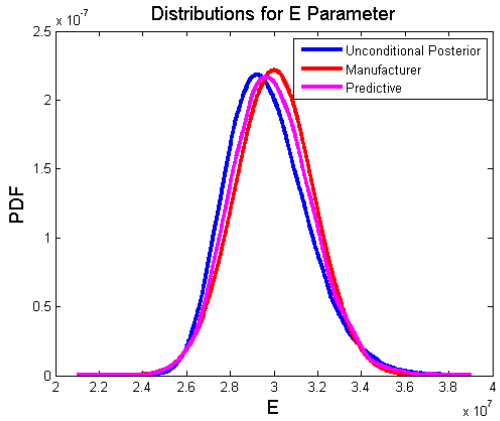
- Weighted average of the model parameters
  - $f(\boldsymbol{\theta})$ → Calibrated unconditional parameter distribution
  - $\hat{f}(\boldsymbol{\theta})$ → Expert opinion distribution (data set 1)
  - $f(\boldsymbol{\theta}|D^V)$ → Predictive distribution

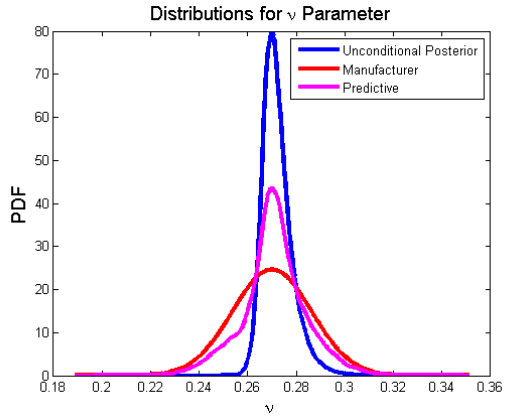
$$f(\theta|D^V) = P(G)f(\theta) + P(\bar{G})\hat{f}(\theta)$$
$$P(\bar{G}) = 1 - P(G)$$

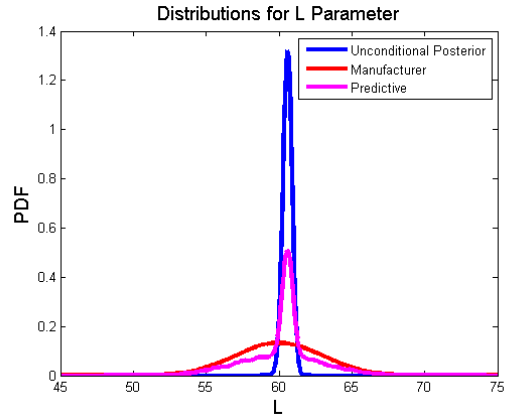
- Uncertainty information on manufacturer data is an important component of the prediction uncertainty

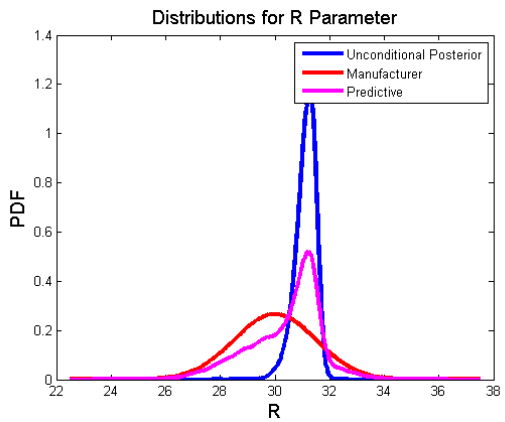
- Two potential options:
  1. Elicit further information from the manufacturer
  2. Consult literature (e.g. National Bureau of Standards: *Development of a Probability Based Load Criterion for American National Standard A58*)

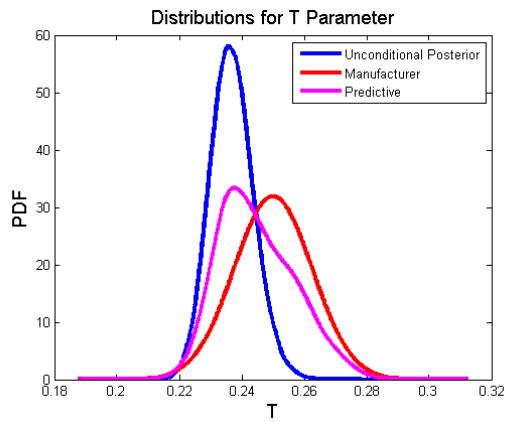
Integrated Parameter Distributions











Conservatism of Tolerance Setting Approach

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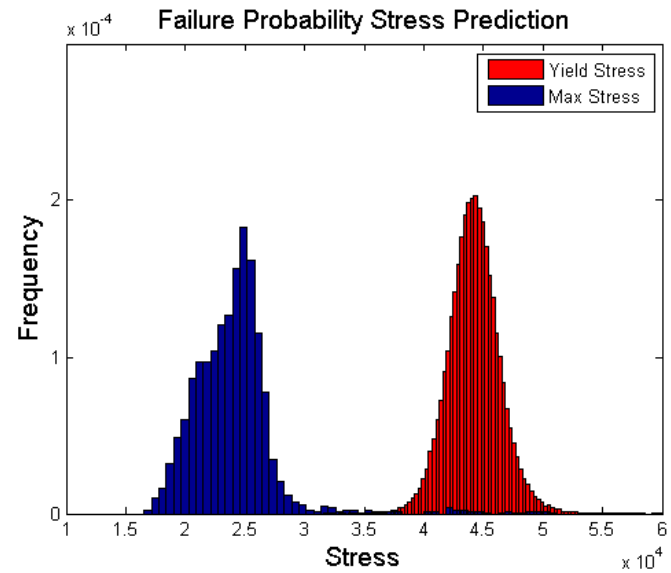
- **Scenario 1:** Model under-predicts observed variability → small tolerance → low model reliability → higher weight on manufacturer data (larger uncertainty)
- **Scenario 2**: Model over-predicts observed variability → high tolerance → high model reliability → higher weight on the large posterior uncertainty

- Thus, in either case, predicted distribution's spread is larger

4. Failure Probability Prediction

- Propagate integrated distribution of θ through the model
- The yield stress is fit to a family of Johnson distributions
- Unconditional yield stress distribution is compared with the maximum stress prediction



Predicted failure probability = 0.0075

Summary

1. Model Calibration
   - Calibrate Johnson distribution parameters that define aleatory variability
   - **Priors**: data sets 2 (E, ν, and t) and 4 (L and R)
   - Update with data set 5
   - Ergodicity assumption (spatial variability and tank-to-tank variability)
2. Model Validation
   - Model reliability metric aimed at epistemic uncertainty
   - Propagate calibration uncertainty and validate on data set 6
3. Integration of Calibration and Validation
   - Weight the calibration results with validation results
   - Poor validation results → use expert opinion (data set 1)
4. Prediction
   - Integrated distribution propagated for failure probability and margin computations