Heteroscedastic Models for Assessing Measurement Uncertainty

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Interlaboratory Studies: The Scenario

- Each of p laboratories makes repeated measurements of m quantities (perhaps corresponding to different concentrations of a chemical analyte).

- The number of measurements made can differ among the laboratories.

- The measurement variability can depend on the material being measured (perhaps as an increasing function of concentration or level).

- The within-laboratory variabilities can differ (often, though, they are assumed to be equal).

Interlaboratory Studies: Some questions

- How should one estimate 'consensus' values of the quantities measured?

- What is the between-laboratory variability (*reproducibility*)?

- What is the within-laboratory variability (*repeatability*)? How do they compare?

- How should one look for outliers?

Why Interlaboratory Studies?

- Interlaboratory studies are primarily performed for one of two reasons:
  1. Validating a measurement method or standard material
  2. Assessing the proficiency of measurement laboratories.

Outline

- A single material measured by multiple laboratories – *one-way random model* (heteroscedastic and unbalanced)
  - Likelihood Analysis
  - Bayesian Model and Credible Regions
  - Examples

- Some results for two-way models.

Dietary Fiber in Apricots
Li and Cardozo (1994)

Lab.	$\bar{x}_i$	s_i^2	n_i
1	25.32	0.37	2
2	26.72	0.62	2
3	27.89	0.35	2
4	27.70	1.85	2
5	27.42	0.61	2
6	24.30	0.21	2
7	27.11	0.37	2
8	27.28	0.09	2
9	25.37	0.08	2

Mean: $\bar{x} = 26.567$

Weighted Means:

$$\begin{aligned} \text{MP} &= 26.472 \\ \text{GD} &= 26.164 \\ \text{ANOVA} &= 26.420 \\ \text{MLE} &= 27.275 \end{aligned}$$

Statistical Framework: One-Way, Unbalanced, Heteroscedastic Random-Effects ANOVA

- Laboratory sample means $\bar{x}_i$ distributed independently normal with mean μ and variance $\sigma^2 + \tau_i^2$, where $\tau_i^2 = \sigma_i^2/n_i$.

- Expected mean for ith laboratory is also normal, with mean μ and variance σ^2.

- Sufficient statistics $\bar{x}_i$ and $t_i^2 = s_i^2/n_i$.

If x_{ij} denotes the jth measurement from the ith lab, then

$$x_{ij} = \mu + b_i + e_{ij},$$

where $b_i \sim \mathrm{N}(0, \sigma^2)$ and $e_{ij} = \mathrm{N}(0, \sigma_i^2)$; mutually independent.

Maximum Likelihood
(Cochran, 1937)

Let $\omega_i = 1/(\sigma^2 + \tau_i^2)$, $\nu_i = n_i - 1$, and determine $\hat{\sigma}$, $\hat{\tau}_i^2$, and $\hat{\mu}$ to satisfy

$$(A_i) \quad \omega_i - \omega_i^2(\bar{x}_i - \mu)^2 + \nu_i\left(\frac{1}{\tau_i^2} - \frac{t_i^2}{\tau_i^4}\right) = 0$$

$$(B) \qquad \boxed{\textstyle\sum_{i=1}^k \omega_i^2(\bar{x}_i - \mu)^2 = \sum_{i=1}^k \omega_i}$$

$$(C) \qquad \mu = \frac{\sum_{i=1}^k \omega_i \bar{x}_i}{\sum_{i=1}^k \omega_i}$$

Note that (B) can have multiple roots. Cochran (1937) proposed setting $\tau_i^2 = t_i^2$ and solving (B) for σ^2, then using (C).

ML Equations

$$\mu = \frac{\sum_{i=1}^{p} \gamma_i \bar{x}_i}{\sum_i \gamma_i} = \frac{\sum_{i=1}^{p} \omega_i \bar{x}_i}{\sum_i \omega_i}$$

$$\sigma^2 = \frac{\sum_{i=1}^{p} \gamma_i \left[(\bar{x}_i - \mu)^2 + \frac{\nu_i t_i^2}{1-\gamma_i} \right]}{\sum_{i=1}^{p} n_i}$$

$$\begin{aligned} &\gamma_i^3 - (a_i + 2)\gamma_i^2 + \\ &[(n_i + 1)a_i + (n_i - 1)b_i + 1]\, \gamma_i \\ &-n_i a_i = 0 \end{aligned}$$

where

$$\gamma_i \equiv \frac{\sigma^2}{\sigma^2 + \tau_i^2}$$

$$a_i \equiv \frac{\sigma^2}{(\bar{x}_i - \mu)^2}$$

and

$$b_i \equiv \frac{t_i^2}{(\bar{x}_i - \mu)^2}.$$

Result #1: Monotone Convergence to Stationary Points of the Likelihood

- For any starting values μ_0, σ_0^2, maximize the likelihood over the weights by solving the cubics. (If there are multiple real roots, choose the one which causes the biggest increase in the likelihood.)

- Let

$$\sigma_1^2 = \frac{\sum_{i=1}^{p} \gamma_i \left[(\bar{x}_i - \mu)^2 + \frac{\nu_i t_i^2}{1-\gamma_i} \right]}{\sum_{i=1}^{p} n_i}$$

$$\mu_1 = \frac{\sum_{i=1}^{p} \gamma_i \bar{x}_i}{\sum_{i=1}^{p} \gamma_i}$$

  solve for new weights, and iterate.

- This iteration, *regardless of starting values*, always converges to a stationary point of the likelihood, and *increases the likelihood at each step.*

Result #2: Location of Stationary Values of the Likelihood

- At a stationary point of the likelihood,

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{p} \gamma_i^2 (\bar{x}_i - \mu)^2}{\sum_{i=1}^{p} \gamma_i}$$

  hence

- *All* of the stationary points of the likelihood $\hat{\mu}$ and $\hat{\sigma}$ are within the rectangle in the (μ, σ) plane given by

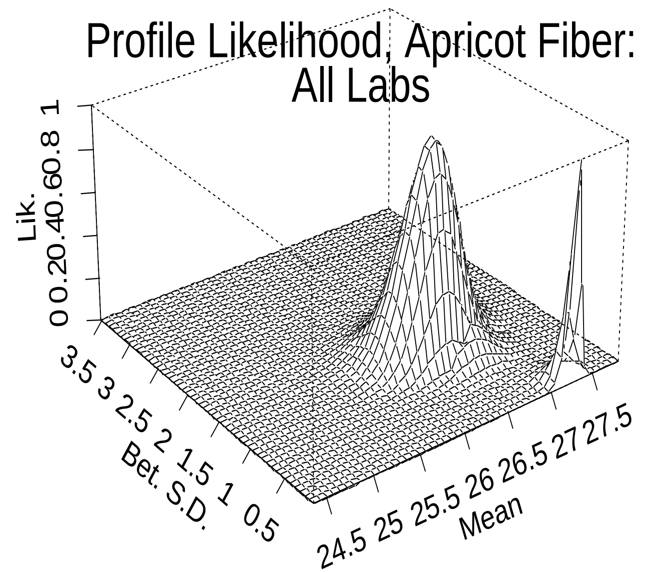
$$\min_i(\bar{x}_i) \leq \tilde{\mu} \leq \max_i(\bar{x}_i)$$

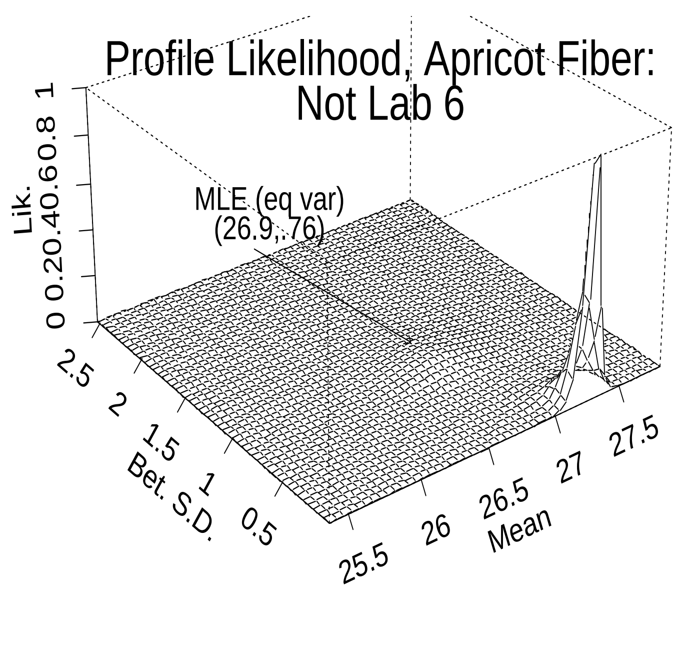
  and

$$0 \leq \tilde{\sigma} \leq \max_i(\bar{x}_i) - \min_i(\bar{x}_i).$$

- After the appropriate location-scale transformation of the data, it is only necessary to search the unit square in the (μ, σ) plane for stationary values.

Lab. 6 an Outlier for Apricot Data





Result #3: Location of the Roots of Cubic Equations for Weights (γ_i)

- Each cubic likelihood equation has one or three roots $\gamma_i \in [0,1]$.

- A necessary condition for three roots is that

$$(\bar{x}_i - \mu)^2 \geq \max(\sigma^2/q_i, t_i^2/h_i),$$

where

$$\begin{aligned} q_i &= -2 - 6\sqrt{n_i}\sin\left\{\frac{1}{3}\left[\sin^{-1}\left(\sqrt{\frac{n_i-1}{n_i}}\right) - \frac{\pi}{2}\right]\right\} \\ &= \frac{8}{27n_i} + O(n_i^{-2}) \end{aligned}$$

and

$$h_i = \frac{(1-q_i)^3}{27(n_i-1)} = \frac{1}{27n_i} + O(n_i^{-2}).$$

- These values q_i and h_i are the smallest for which this is necessary.

Hierarchical Model With Noninformative Priors

$i = 1, \ldots, p$ indexes laboratories

$j = 1, \ldots, n_i$ indexes measurements

$$\begin{aligned} p(x_{ij}|\delta_i, \sigma_i^2) &= \mathsf{N}\,(\delta_i, \sigma_i^2) \\ p(\sigma_i) &\propto 1/\sigma_i \\ p(\delta_i|\mu, \sigma^2) &= \mathsf{N}\,(\mu, \sigma^2) \\ p(\mu) &= 1 \\ p(\sigma) &= 1 \end{aligned}$$

A Useful Probability Density

Let T_ν and Z denote independent Student-t and standard normal random variables, and assume that $\psi \geq 0$ and $\nu > 0$. Then

$$U = T_\nu + Z\sqrt{\frac{\psi}{2}}$$

has density

$$f_\nu\left(u;\psi\right) \equiv \frac{1}{\Gamma\left(\nu/2\right)\sqrt{\pi}}\int_0^\infty \frac{y^{(\nu+1)/2-1}e^{-y\left[1+\frac{u^2}{\psi y+\nu}\right]}}{\sqrt{\psi y+\nu}}dy.$$

Posterior of (μ, σ)

- Assume $\delta_i \sim \mathsf{N}(\mu, \sigma^2)$, $\sigma \sim p(\sigma)$, $p(\mu) = 1$, $p(\sigma_i) = 1/\sigma_i$.

- Then the posterior of (μ, σ) is

$$p(\mu, \sigma | \{x_{ij}\}) \propto p(\sigma) \prod_{i=1}^{p} \frac{1}{t_i} f_{n_i - 1} \left[\frac{\bar{x}_i - \mu}{t_i}; \frac{2\sigma^2}{t_i^2} \right].$$

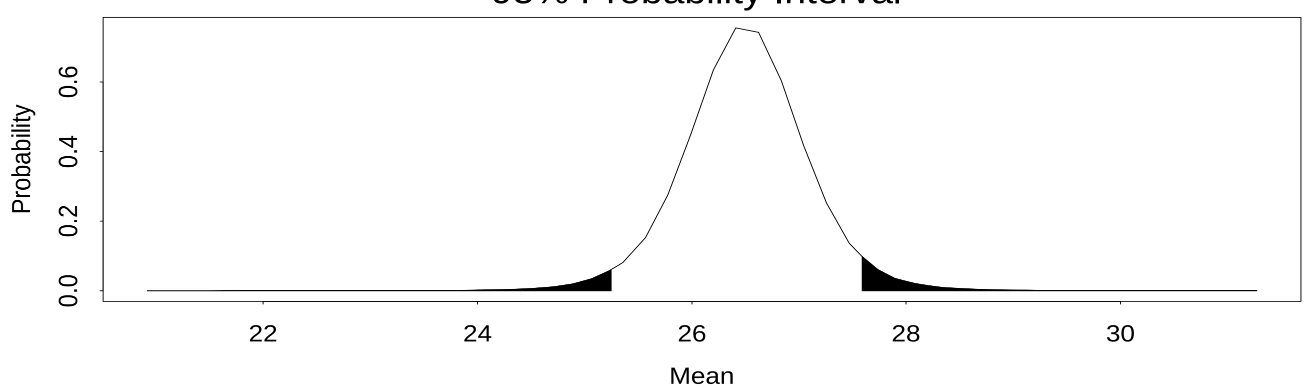
- The posterior of μ given $\sigma = 0$ is a product of scaled t-densities centered at the $\bar{x}_i$, since

$$\frac{1}{t_i} f_{n_i - 1} \left[\frac{\bar{x}_i - \mu}{t_i}; 0 \right] = \frac{1}{t_i} T'_{n_i - 1} \left(\frac{\bar{x}_i - \mu}{t_i} \right).$$

- We will take $p(\sigma) = 1$, though an arbitrary proper prior does not introduce additional difficulties.

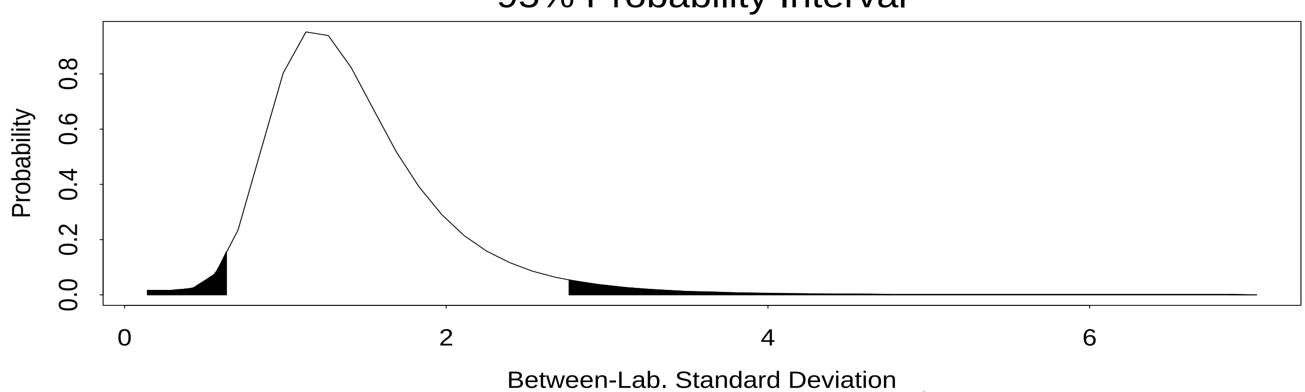
Approximate Confidence Intervals: Apricot Fiber Data

Marginal Posterior of Mean With
95% Probability Interval



Post. mean = 26.499 Post. S.D. = 0.587 25.246 < mean < 27.588

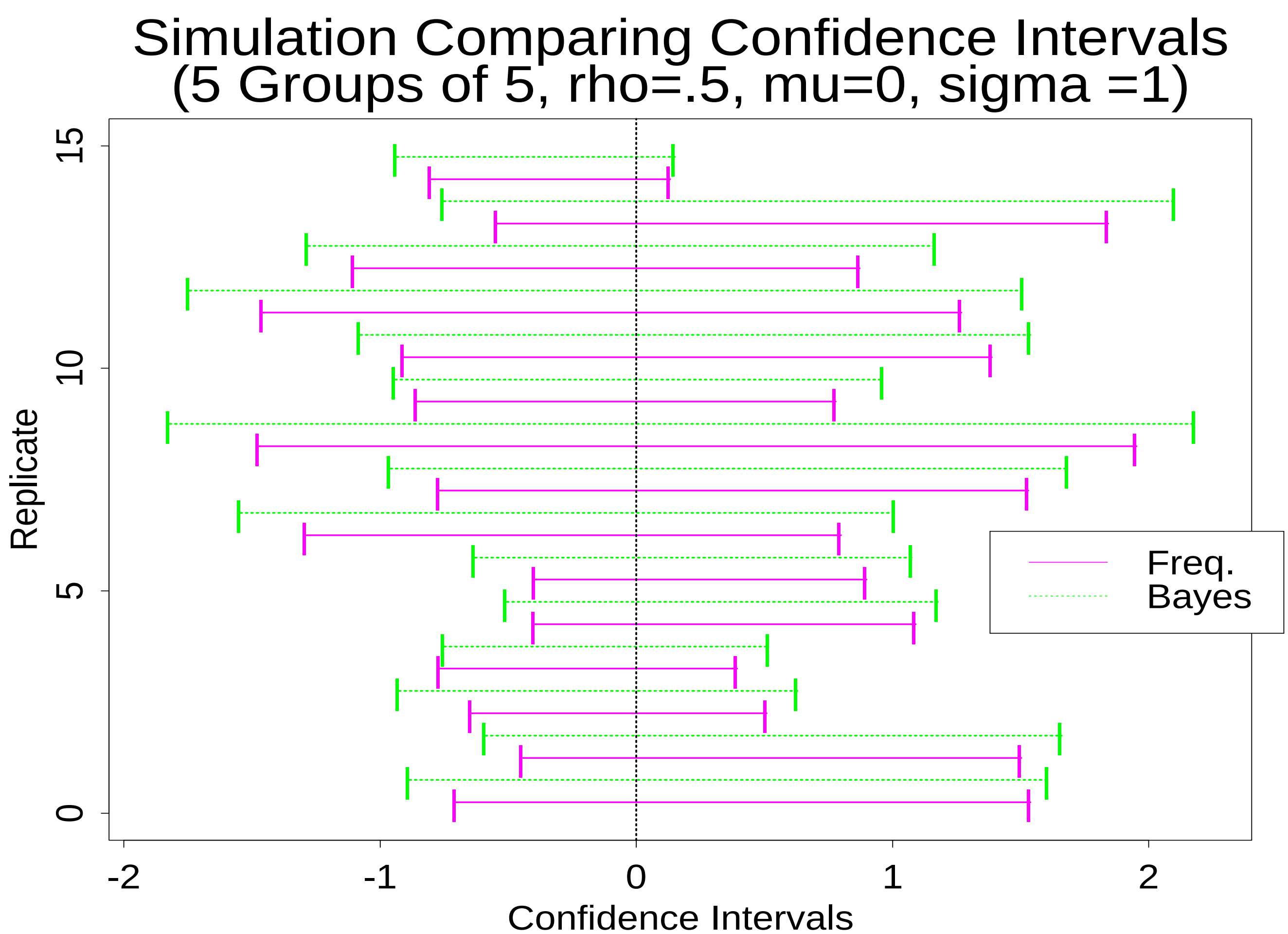
Marginal Posterior of Between-Lab. S.D. With
95% Probability Interval



Post. mean = 1.438 Post. S.D. = 0.558 0.633 < sigma < 2.763

Small Simulation Comparing Bayesian and Frequentist Intervals

$$\begin{aligned}\mu &= 0\\ \sigma_i &= \sigma_e\\ \sigma^2+\sigma_e^2 &= 1\\ \rho &= \sigma^2/(\sigma_e^2+\sigma^2) = 1/2\end{aligned}$$



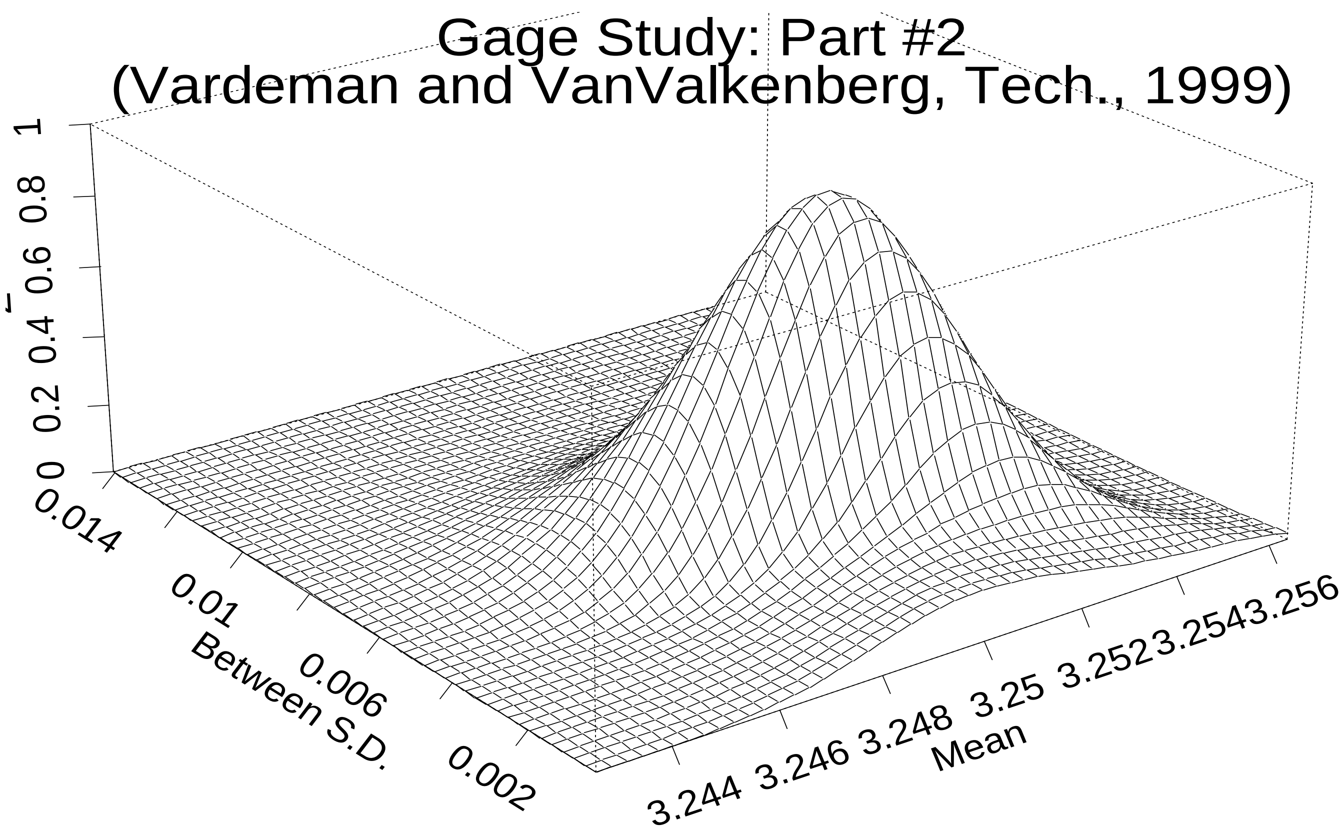
A Gage Study Example: Vardeman and VanValkenberg, Tech. (1999)

Rep.	Operator				
1	3.258	3.254	3.256	2.249	3.241
2	3.254	3.247	3.257	3.238	3.250
3	3.258	3.239	3.245	3.240	3.254

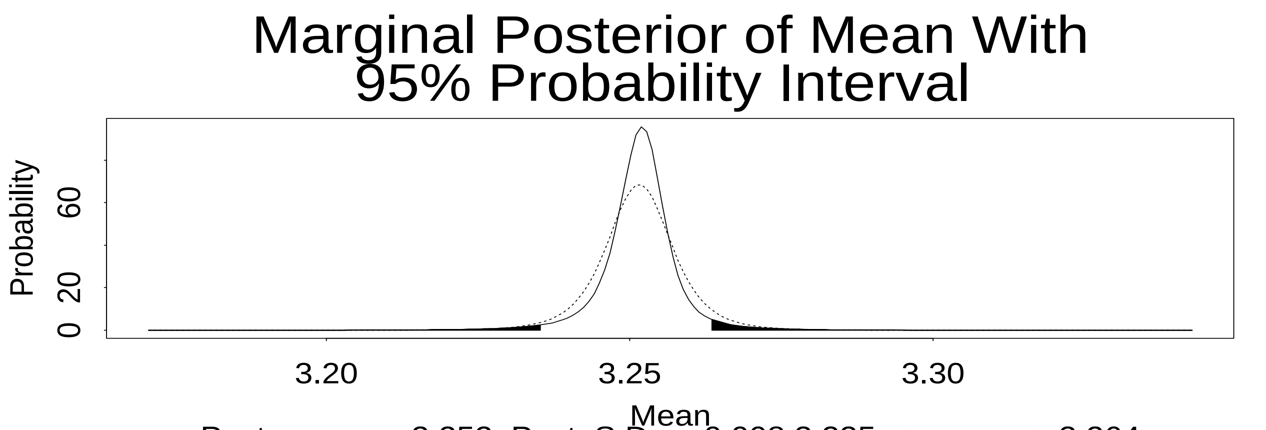
– Single part, 5 operators, 3 replicates

– Note tied values for Operator 1

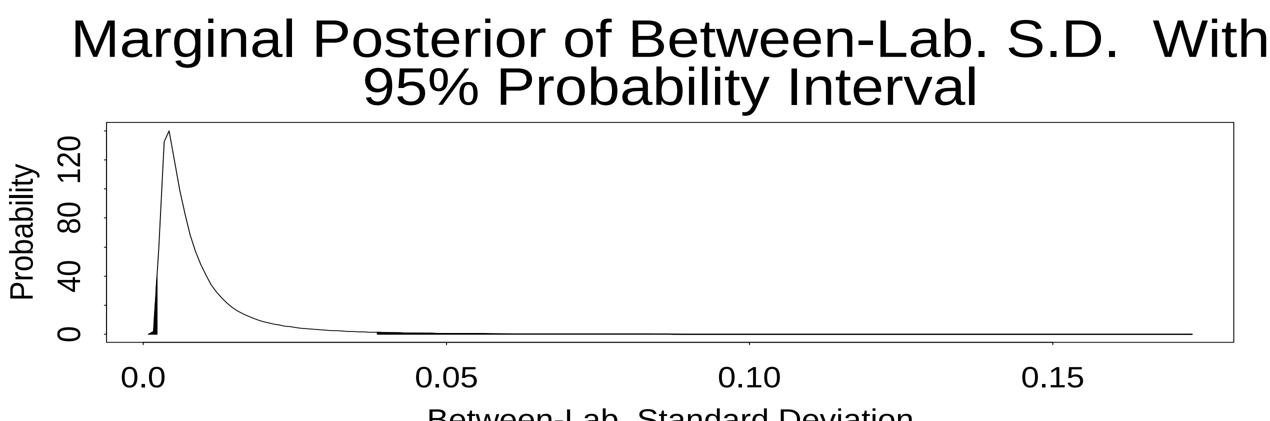
Profile Likelihood



Marginal Posteriors: Vardeman and VanValkenberg Gage Study, Part#2



Post. mean = 3.252 Post. S.D. = 0.008 3.235 < mean < 3.264



Post. mean = 0.01 Post. S.D. = 0.012 0.002 < sigma < 0.039

A Two-Way Mixed Model
(Heteroscedastic, no Interaction)

$$x_{ijk} = \theta_k + \delta_i + e_{ijk},$$

- $i = 1, \ldots, p$ Laboratories
- $j = 1, \ldots, n_i$ Replicates
- $k = 1, \ldots, m$ Materials

$$\delta_i \sim \mathrm{N}\,(0, \sigma^2)$$

$$e_{ijk} \sim \mathrm{N}\,(0, \sigma_i^2)$$

Some notation: $\tau_i^2 \equiv \sigma_i^2/(n_i m)$, $\nu_i \equiv n_i m - 1$.

ML Equations

$$\theta_k - \bar{\theta} \equiv \phi_k = \frac{\sum_{i=1}^{p}(\bar{x}_{i\cdot k} - \bar{x}_{i\cdot\cdot})/\tau_i^2}{\sum_{i=1}^{p} 1/\tau_i^2}$$

$$\bar{\theta} = \frac{\sum_{i=1}^{p} \gamma_i \bar{x}_{i\cdot\cdot}}{\sum_{i=1}^{p} \gamma_i}$$

$$\sigma^2 = \frac{\sum_{i=1}^{p} \gamma_i \left[(\bar{x}_{i\cdot\cdot} - \bar{\theta})^2 + \frac{\nu_i t_i^2}{1-\gamma_i}\right]}{\sum_{i=1}^{p} n_i}$$

Where $\tau_i^2 \equiv \sigma_i^2/(n_i m)$, $\nu_i \equiv mn_i - 1$, $\gamma_i \equiv \sigma^2/(\sigma^2 + \tau_i^2)$, and

$$t_i^2 \equiv \frac{\sum_{j,k}(x_{ijk} - \bar{x}_{i\cdot k})^2 + n_i \sum_k (\bar{x}_{i\cdot k} - \bar{x}_{i\cdot\cdot} - \phi_k)^2}{\nu_i n_i m}$$

ML Equations (Cont'd)

The weights $\{\gamma_i\}_{i=1}^{p}$ are roots of the cubic equations

$$\gamma_i^3 - (a_i + 2)\gamma_i^2 + \\ [(n_i m + 1)a_i + \nu_i b_i + 1]\,\gamma_i - \\ n_i a_i = 0$$

where

$$a_i \equiv \frac{\sigma^2}{(\bar{x}_{i\cdot\cdot} - \bar{\theta})^2}$$

and

$$b_i \equiv \frac{t_i^2}{(\bar{x}_{i\cdot\cdot} - \bar{\theta})^2}.$$

An ML Iteration

1. Begin with estimates $\left\{\gamma_i^{(s)}\right\}$.

2. Calculate the following:

$$\begin{aligned}
\phi_k^{(s+1)} &= \frac{\sum_{i=1}^{p}(\bar{x}_{i\cdot k}-\bar{x}_{i\cdot\cdot})/\tau_i^{2(s)}}{\sum_{i=1}^{p} 1/\tau_i^{2(s)}} \\
\bar{\theta}^{(s+1)} &= \frac{\sum_{i=1}^{p}\gamma_i^{(s)}\bar{x}_{i\cdot\cdot}}{\sum_{i=1}^{p}\gamma_i^{(s)}} \\
\sigma^2_{(s+1)} &= \frac{\sum_{i=1}^{p}\gamma_i^{(s)}\left[(\bar{x}_{i\cdot\cdot}-\bar{\theta})^2+\frac{\nu_i t_i^2}{1-\gamma_i^{(s)}}\right]}{\sum_{i=1}^{p} n_i}
\end{aligned}$$

3. Note that if the ϕ_k are constrained to satisfy the above ML equation, then

$$t_i^2 = \frac{\sum_{j,k}(x_{ijk}-\bar{x}_{i\cdot\cdot})^2 - \sum_k \phi_k^2/m}{n_i \nu_i m}$$

4. Solve the cubics for new estimates $\gamma_i^{(s+1)}$, and iterate.

Some Theoretical Results for Two-Way Mixed Model

The one-way results discussed earlier generalize:

- Monotone convergence
- All stationary values of likelihood in box in $(\mu, \sigma, \sum_k \phi_k^2)$ space.
- Exactly one weight $\gamma_i \in [0, 1]$, unless ith lab an outlier and n_i small
- Variances cannot be negative at solution to likelihood equation.

Summary

- A reparametrization of the likelihood in the one-way heteroscedastic model leads to new insights in likelihood and Bayesian analyses.

- Allowing "within" (*repeatability*) variances to differ can reduce the estimated "between" (*repeatability*) variance.

- Many of these results carry over to two-way models; this work is ongoing.