LAUNCH AND DEMONSTRATION OF THE NIST HOMOGENEITY ASSESSOR



By: Luke Benz Mentor: Dr. Antonio Possolo Statistical Engineering Division Information Technology Laboratory NIST SURF Summer 2018



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M&M's: A Motivating Example

- Suppose Mars, Inc wants to see if their bags are homogeneous with respect to the fraction of Red M&M's in each bag.
- Randomly sample several bags off the assembly line—Impossible to look at every bag!
 - Measurand = Fraction of Red M&M's
 - Sampling Factor = Bag
- More interest in between-bag variability than specific fractions of Red M&M's



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Reference Materials

- Reference Materials: calibration of measuring instruments and validation of experimental results.
- Developing and certifying reference materials is a core part of the NIST mission.
- Examples of NIST SRMs
 - Chromium-Nickel-Molybdenum Steel (SRM 139b)
 - Peanut Butter (SRM 2387)
 - Lake Michigan Fish Tissue (SRM 1947)



https://gizmodo.com/the-761-peanut-butter-and-other-insanely-expensive-gov-1690984965

Homogeneity

- Reference materials distributed in distinct portions of batch called "units".
- Unit Examples: Box, Bottle, Canister, etc.
- Reference material is homogeneous if measurement results from different units are statistically indistinguishable (ISO, 2017)
- Most materials exhibit some level of heterogeneity:
 - Recognized and expressed in the uncertainty associated with the reference value.

NIST Homogeneity Assessor (NIHOMA)

- R/Shiny App
- Estimates heterogeneity and illustrates its sources.
- Designed for scientists to understand variability in their data.



NIHOMA Demonstration

- Methane fraction (cmol/mol) in synthetic mixture mimicking Natural Gas
- 5 replicate determinations for 10 cylinders

Amount_Fraction (cmol/mol)	Cylinder
85.95544434	D520472
85.94890755	D520472
85.95284753	D520472
85.95239981	D520472
85.94040077	D520472
85.97198209	H95396
85.96831081	H95396
85.97619063	H95396
85.98299593	H95396
85.96052053	H95396
85.96098584	VSL190663
85.95435998	VSL190663
85.97307355	VSL190663
85.97208862	VSL190663
85.969492	VSL190663
85.9779247	D520467
85.96225521	D520467

Linear Gaussian Random Effects Model

■ The engine behind the NIHOMA is linear, Gaussian random effects model.



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Testing for Homogeneity

- Are the between-bottle differences significantly larger than the within-bottle differences?
- Is variance of bottle effects both statistically significant and substantively?
- When there is statistically significant heterogeneity:
 - Split the material into less heterogeneous materials
 - Fold the resulting contribution into the overall uncertainty

	_	term	group	estimate	2.5 %	97.5 %	std.uncertainty	
1	Si	gma Cylinder	Cylinder	0.01062	0.004945	0.01595		
2	Sigma	Within_Group	Residual	0.009104	0.007188	0.01099		
3		Measurand	Fixed Effects	85.96	85.95	85.97	0.003598	

NIHOMA—Flexibility







- Data Entry as Single Measurement Result Per Unit
 - Allows user to factor in uncertainty other than bottle dispersions before running the analysis.
 - Allows user to perform analysis when only a single replicate is available per bottle.
- Multi-Factor Sampling Designs
 - Allows for analysis of studies with more complex sampling structures, with multiple factors nested within one another.
 - Customizable Group Subset Plot, with faceting by second sampling factor if desired.

NIHOMA—Ready to Use and to Grow

- Available for use by NIST scientists NOW on the internal NIST Web
- User's Manual (40+ pages) with explanations and examples
- Extensible and modifiable upon user feedback
- Soon to be made freely available worldwide
 - NIST GitHub
 - R Package

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Questions?