Sampling-Based Methods for Uncertainty and Sensitivity Analysis

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Sampling-Based Methods for Uncertainty and Sensitivity Analysis

- Involve generation and exploration of mapping from analysis inputs to analysis results

- Analysis input: $\boldsymbol{x} = [x_1, x_2 \ldots, x_{nX}]$

- Analysis results: $\mathbf{y}(\mathbf{x}) = [y_1(\boldsymbol{x}), y_2(\boldsymbol{x}), \ldots, y_{nY}(\boldsymbol{x})]$

- Two Questions
  - What is the uncertainty in $\boldsymbol{y}(\boldsymbol{x})$ given the uncertainty in $\boldsymbol{x}$?
  - How important are the individual elements of $\boldsymbol{x}$ with respect to the uncertainty in $\boldsymbol{y}(\boldsymbol{x})$?

Uncertainty in Analysis Input

- Uncertainty in ***y*** derives from uncertainty in ***x***
- Assumption: Appropriate value for ***y*** obtained if appropriate value for ***x*** used
- Problem: Impossible to specify appropriate value for ***x*** unambiguously
- Many possible values of ***x*** of varying levels of plausibility
- Uncertainty with respect to ***x***
  - Designated subjective or epistemic uncertainty
  - Characterized by distributions $D_1, D_2, \ldots, D_{nX}$ assigned to elements $x_1, x_2, \ldots, x_{nX}$ of ***x***

Propagation of Uncertainty

- Generate sample: $\boldsymbol{x}_k$, $k = 1,2,\ldots,nS$
- Evaluate $\boldsymbol{y}$: $\boldsymbol{y}(\boldsymbol{x}_k)$, $k = 1,2,\ldots,\mathrm{nS}$
- Resultant mapping: $[\boldsymbol{x}_k, \boldsymbol{y}_k(\boldsymbol{x}_k)]$, $k = 1,2,\ldots nS$
- Mapping forms basis for
  - Uncertainty analysis (distribution functions, box plots…)
  - Sensitivity analysis (scatterplots, regression analysis,…)

Components of Sampling-Based Uncertainty/Sensitivity Analysis

- Characterization of uncertainty in $\boldsymbol{x}$ (i.e., definition of $D_1, D_2, \ldots, D_{nX}$)

- Generation of sample from $\boldsymbol{x}$ (i.e., generation of $\boldsymbol{x}_k$, $k = 1,2,\ldots,nS$, in consistency with $D_1, D_2, \ldots, D_{nX}$)

- Propagation of sample through analysis (i.e., generation of mapping $[\boldsymbol{x}_k, \boldsymbol{y}(\boldsymbol{x}_k)]$, $k = 1,2,\ldots,nS$)

- Presentation of uncertainty analysis results (i.e., approximations to the distributions of the elements of $\boldsymbol{y}$ obtained from $\boldsymbol{y}(\boldsymbol{x}_k)$, $k = 1,2,\ldots,nS$)

- Determination of sensitivity analysis results (i.e., exploration of the mapping $[\boldsymbol{x}_k, \boldsymbol{y}(\boldsymbol{x}_k)]$, $k = 1,2,\ldots,nS$)

Example Analysis: Two-Phase Fluid Flow

- Context: Radioactive waste disposal facility in bedded salt
- Mathematics: System of nonlinear partial differential equations
- Numerics: Finite difference procedure on two-dimensional grid
- Uncertainties: 31 uncertain inputs (i.e., $nX = 31$)

Example Analysis: Uncertain Inputs

- Uncertain inputs
  - *ANRGSSAT*-Residual gas saturation in anhydrite
  - *BHPRM*-Logarithm of borehole permeability
  - *BPCOMP*-Logarithm of bulk compressibility of brine pocket
    Correlation: –0.75 rank correlation with *BPPRM*

    ...
  - *WRBRNSAT*-Residual brine saturation in waste
  - WRGSSAT-Residual gas saturation in waste

- Vector representation

  $\boldsymbol{x} = [x_1, x_2, \ldots, x_{nX}]$, $nX = 31$

  $= [ANRGSSAT, BHPRM, \ldots, WRGSSAT]$

Example Analysis: Results

- Many analysis results
  - Pressure
  - Brine and gas saturations
  - Gas production due to corrosion and microbial degradation of cellulose
  - Brine and gas flows across specified boundaries
  - and many more

- $\boldsymbol{y}(\boldsymbol{x}) = [y_1(\boldsymbol{x}), y_2(\boldsymbol{x}), \ldots, y_{nY}(\boldsymbol{x})]$
  - nY potentially very large
  - Elements $y_j(\boldsymbol{x})$ of $\boldsymbol{y}(\boldsymbol{x})$ functions of time and space, i.e., $y_j(x, y, t, \boldsymbol{x})$

Characterization of Uncertainty in ***x***

- Corresponds to definition of $D_1, D_2, \ldots, D_{nX}$
- Most important part of sampling-based uncertainty/sensitivity analysis
- Determines both
  - Uncertainty in ***y***
  - Sensitivity of ***y*** to elements of ***x***
- $D_1, D_2, \ldots, D_{nX}$ typically defined through expert review/elicitation process
- Extensive literature available
- Not primary focus of this presentation

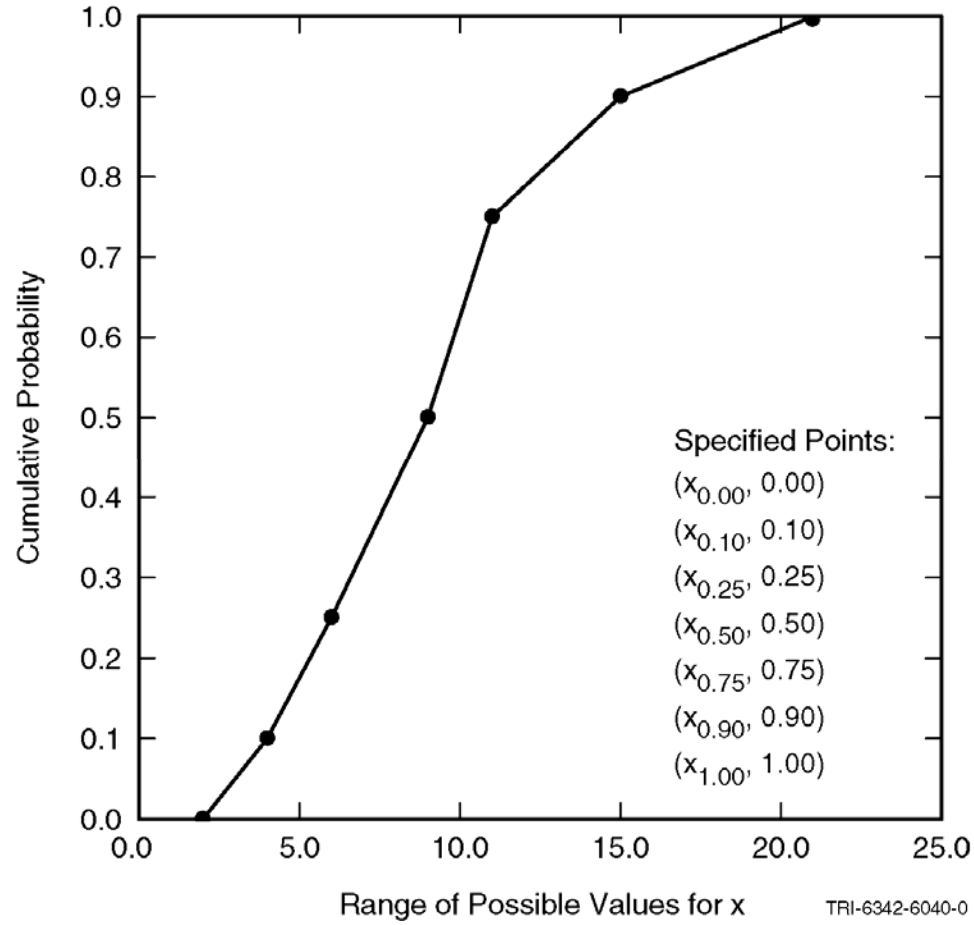
Observation on the Characterization of Uncertainty in $\boldsymbol{x}$

- Understand type of information characterized by $D_1, D_2, \ldots, D_{nX}$
  - Degree of belief with respect to where appropriate value of each element of $\boldsymbol{x}$ is located for use in analysis

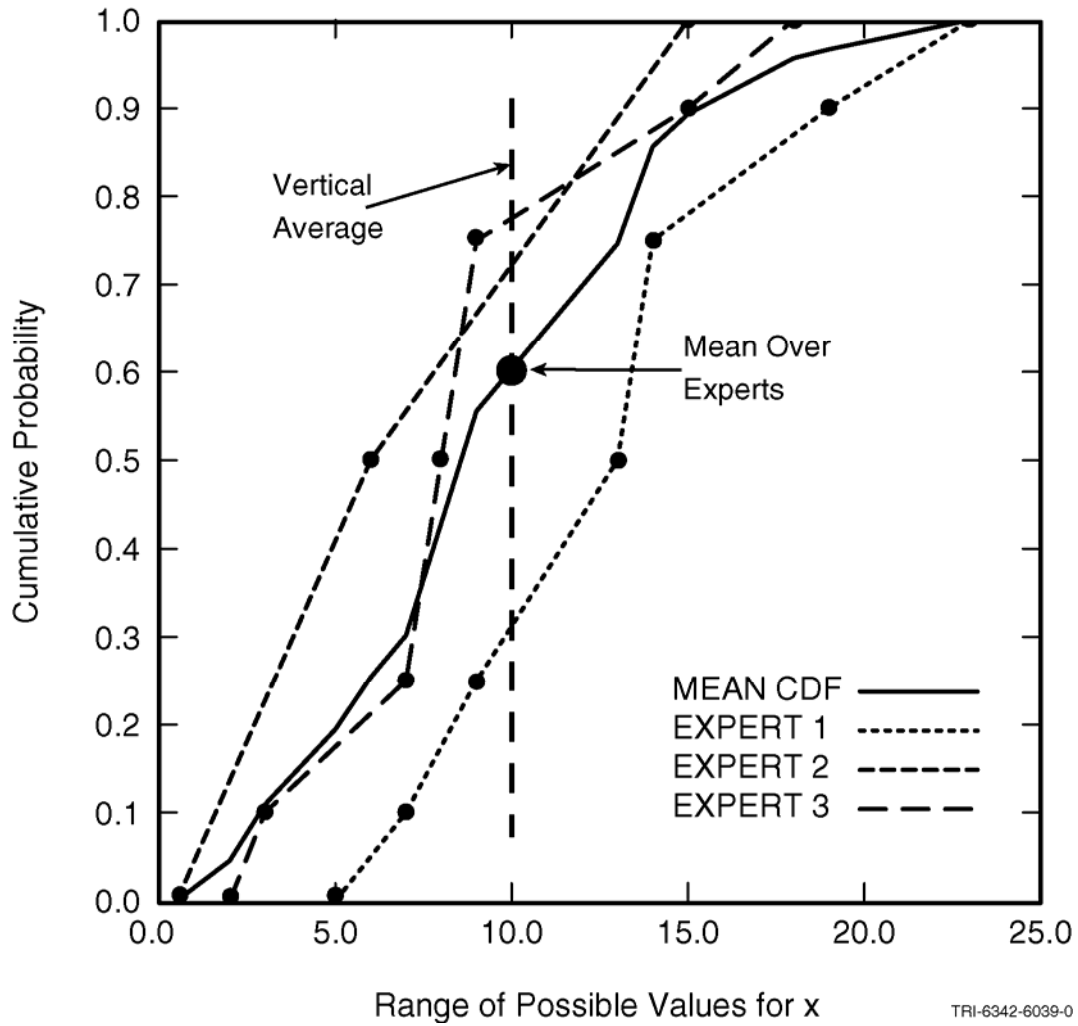
- Do not confuse uncertainty with spatial, temporal or experimental variability
  - If analysis uses a spatially or temporally averaged value for x_j, then D_j should characterize uncertainty in this average, <u>not</u> the variability that is averaged over
  - Similarly, experimental variability is not the same as uncertainty in an analysis input derived from variable experimental outcomes

Possible Construction Procedure for D_j

- Specify
  - Min and max values
  - Median
  - Quartiles
  - Additional quantiles
- Document rationale



Possible Construction Procedure for D_j with Multiple Experts



Observations on Construction of $D_1, D_2, \ldots, D_{nX}$

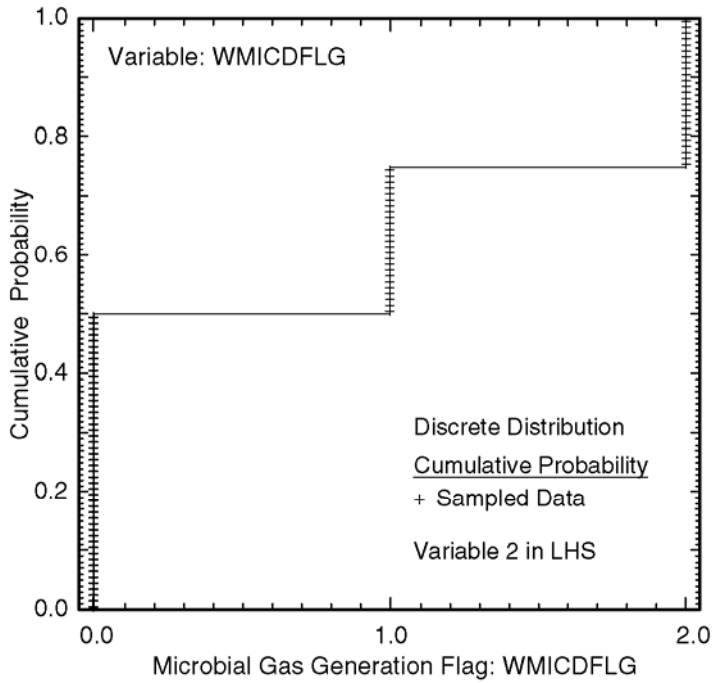
- Can be most expensive and important part of analysis
- Care and effort dependent on
  - Purpose of analysis
  - Time and resources available
- Exploratory analysis
  - Crude specifications (e.g., uniform and loguniform)
  - Will probably reveal dominant variables
- Analysis that forms basis for important decisions
  - Care required in construction of $D_1, D_2, \ldots, D_{nX}$
  - $D_1, D_2, \ldots, D_{nX}$ influence both uncertainty and sensitivity analysis results

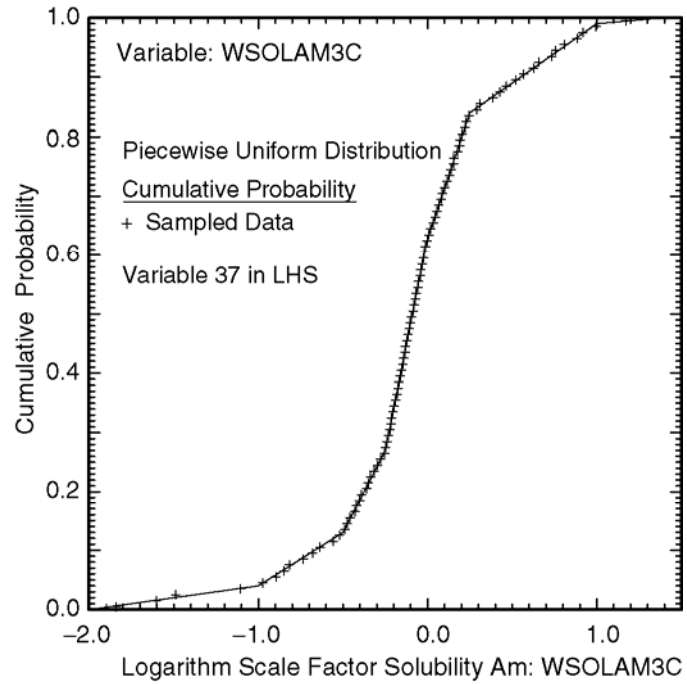
Possible Analysis Strategy

- Perform initial (exploratory) analysis
  - Crude definitions for $D_1, D_2, \ldots, D_{nX}$
  - Identify important variables with sensitivity analysis
- Characterize uncertainty in important variables
- Perform second analysis
  - Presentation or decision-aiding analysis
  - Use refined distributions for important variables

Example Analysis: Distributions

- Distributions developed from 31 uncertain variables
- Examples below





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Sampling Procedures: Random Sampling

- Random sample: $\boldsymbol{x}_k = [x_{1k}, x_{2k}, \ldots, x_{nX,k}]$, $k = 1,2,\ldots,nR$

- Sample elements (i.e., $\boldsymbol{x}_k$'s) from different regions of sample space occur in direct relationship to the probability of these regions

- Each sample element selected independently of all other sample elements

Sampling Procedures: Importance Sampling

- Importance sample: $\boldsymbol{x}_k = [x_{1k}, x_{2k}, \ldots, x_{nX,k}]$, $k = 1,2,\ldots,nS$

- Sample space divided into strata $S_1, S_2, \ldots, S_{nS}$ which
  - Typically have unequal probabilities
  - Assure inclusion of specific regions of sample space in analysis

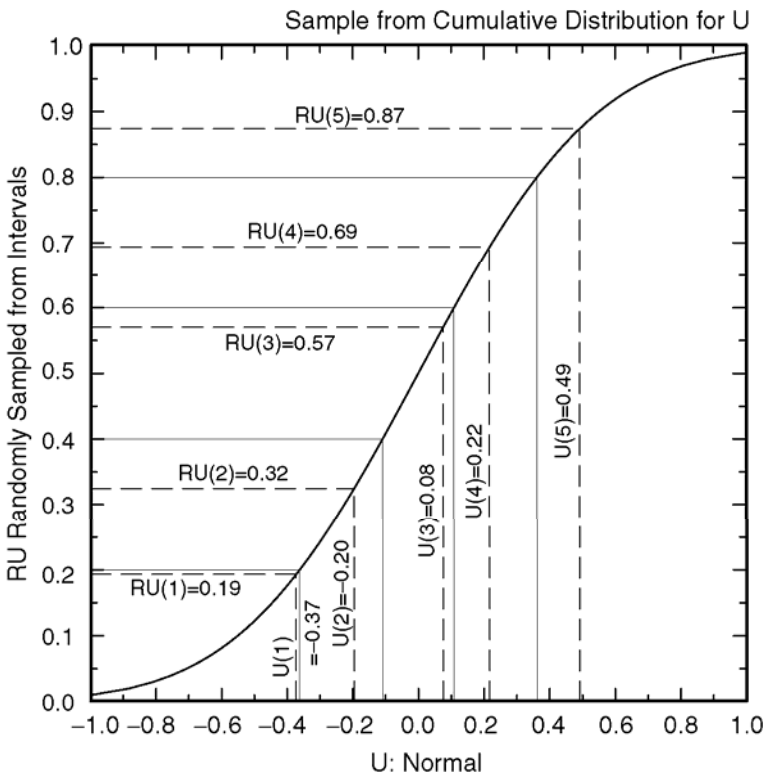
- Sample element $\boldsymbol{x}_k$ randomly sampled from strata S_k

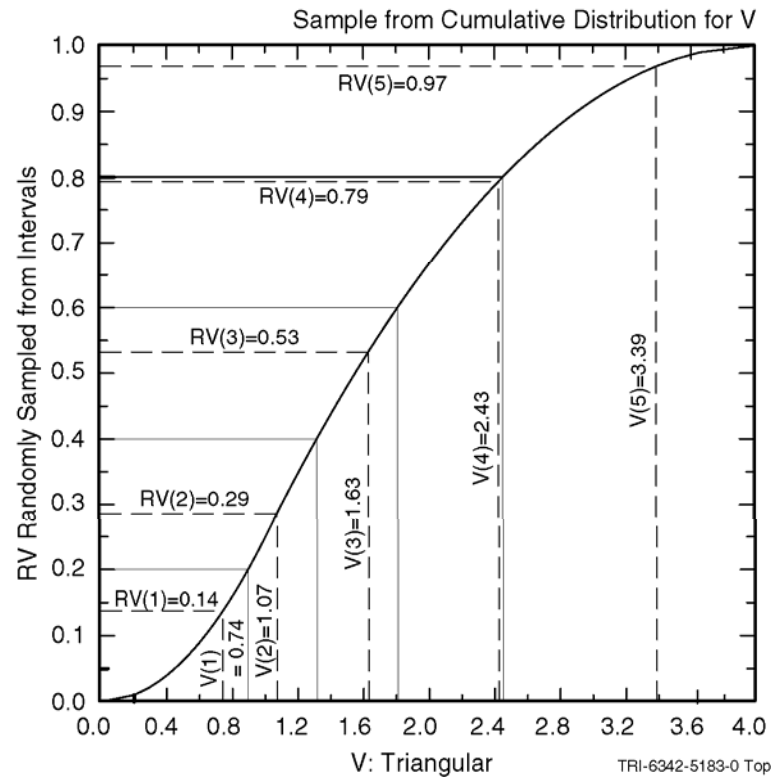
Sampling Procedures: Latin Hypercube Sampling

- Latin hypercube sample (LHS): $\boldsymbol{x}_k = [x_{1k}, x_{2k}, \ldots, x_{nX,k}]$, $k = 1,2,\ldots,nLHS$

- Generation of sample
  - Range of each x divided in $nLHS$ intervals of equal probability
  - Value for x_j (i.e., x_{jk}) randomly selected from each interval
  - Values for x_1 randomly paired without replacement with values for x_2 to produce $nLHS$ pairs
  - Preceding pairs randomly combined without replacement with values for x_3 to produce $nLHS$ triples
  - Process continues through all variables to produce $nLHS$ sample elements

Latin Hypercube Sampling: Example

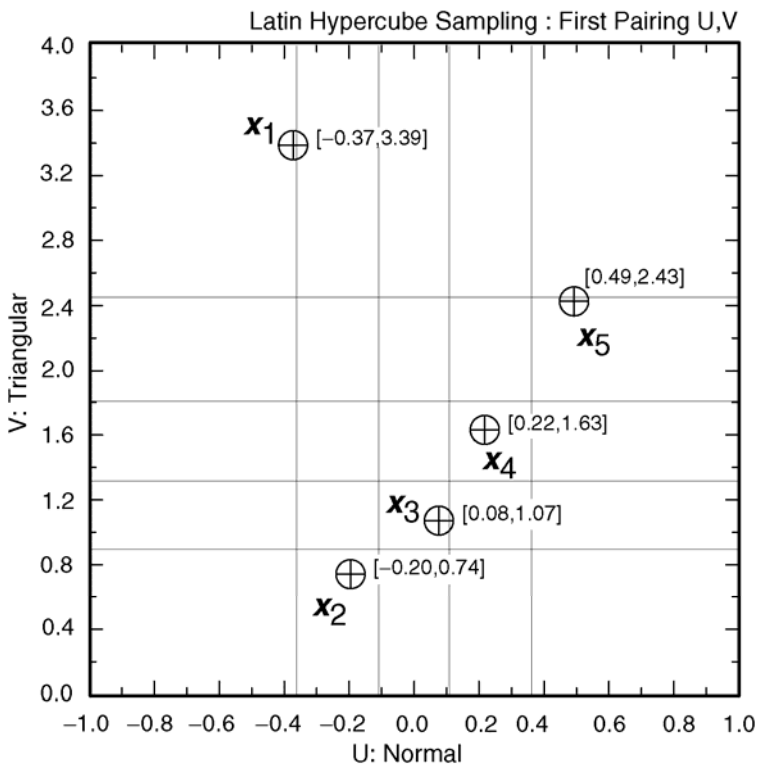


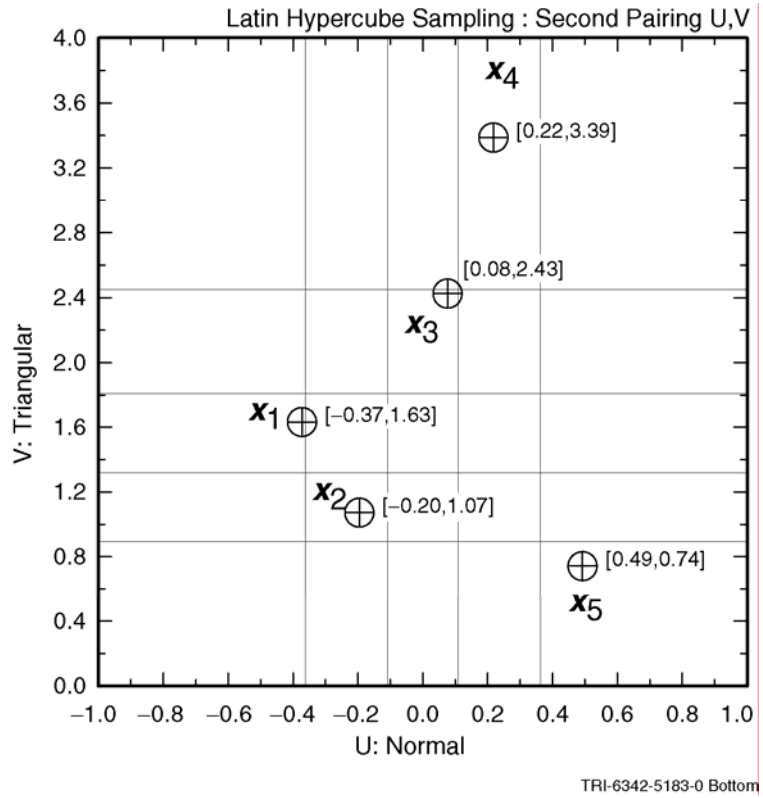


RU_1: $U_1 = -0.37$
RU_2: $U_2 = -0.20$
…
RU_5: $U_5 = 0.49$

RV_1: $V_1 = 0.74$
RV_2: $V_2 = 1.07$
...
RV_3: $V_5 = 3.39$

Latin Hypercube Sampling: Example (cont)





$\boldsymbol{x}_1 = [U_1, V_5]$
$\boldsymbol{x}_2 = [U_2, V_1]$
…
$\boldsymbol{x}_5 = [U_5, V_4]$

$\boldsymbol{x}_1 = [U_1, V_3]$
$\boldsymbol{x}_2 = [U_2, V_2]$
…
$\boldsymbol{x}_5 = [U_5, V_1]$

Comparison of Sampling Techniques

- Random sampling preferred when sufficiently large samples are possible
  - Easy to implement
  - Easy to explain
  - Unbiased estimates for means, variances and distribution functions
  - Sufficiently large samples may not be possible

- Importance sampling
  - Used when random sampling not computationally feasible for estimation of extreme quantiles
  - Development of strata and strata probabilities often challenging
  - Requires *a priori* knowledge about problem
  - Event trees are algorithms for defining importance sampling

Comparison of Sampling Techniques (cont)

- Latin hypercube sampling
  - Unbiased estimates for means and distribution functions
  - Dense stratification across range of each variable
  - Used when large samples not computationally practicable and estimation of high quantiles not required
  - Preceding is typically the case in uncertainty/sensitivity analyses to assess effects of subjective uncertainty
  - Uncertainty/sensitivity results robust with relatively small sample sizes (e.g., *nLHS* = 50 to 200)

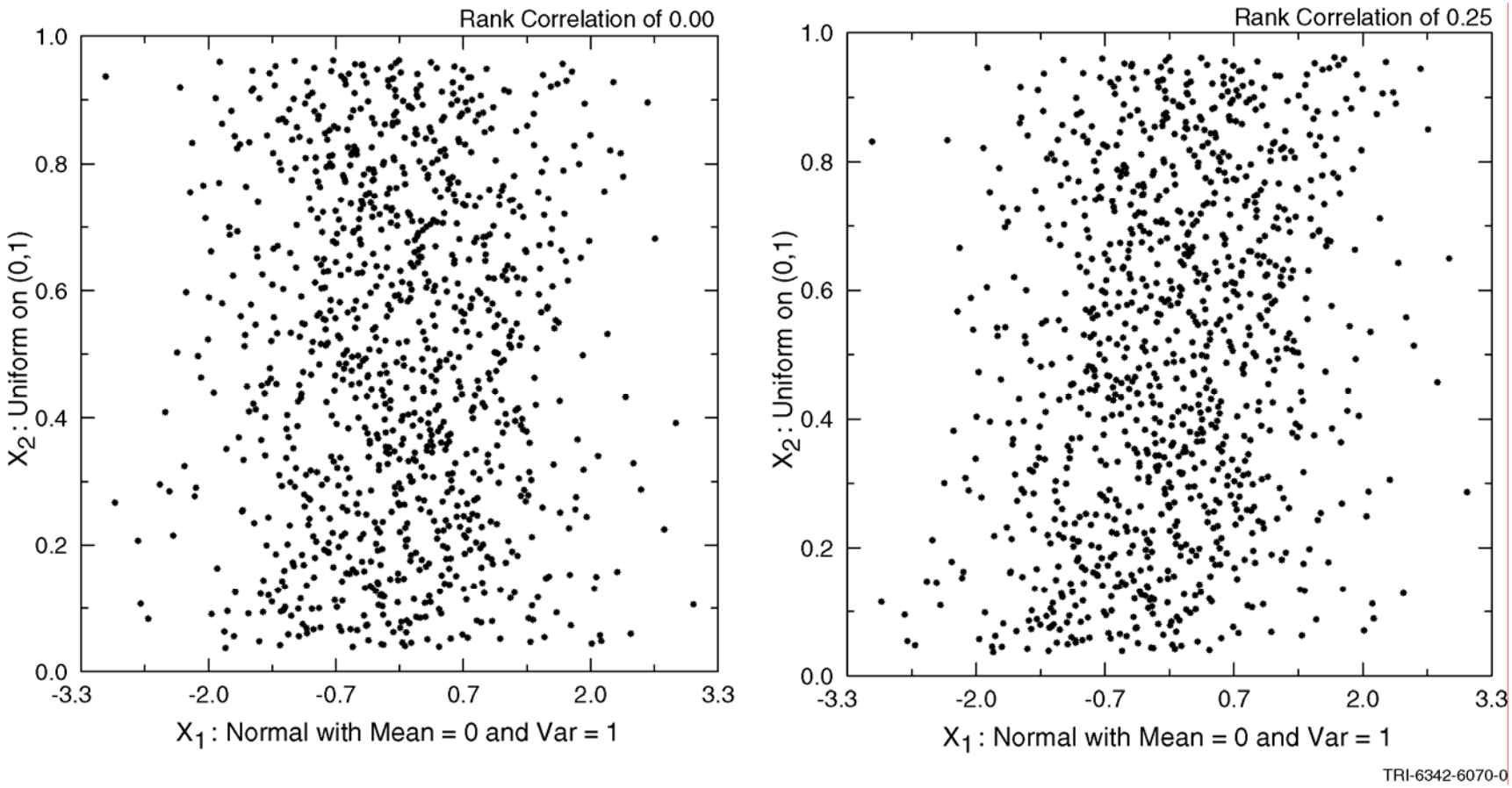
Random and LH Sampling: Correlation Control

- Correlation control important
  - Correlated variables should have appropriate correlations
  - Uncorrelated variables should have correlations close to zero

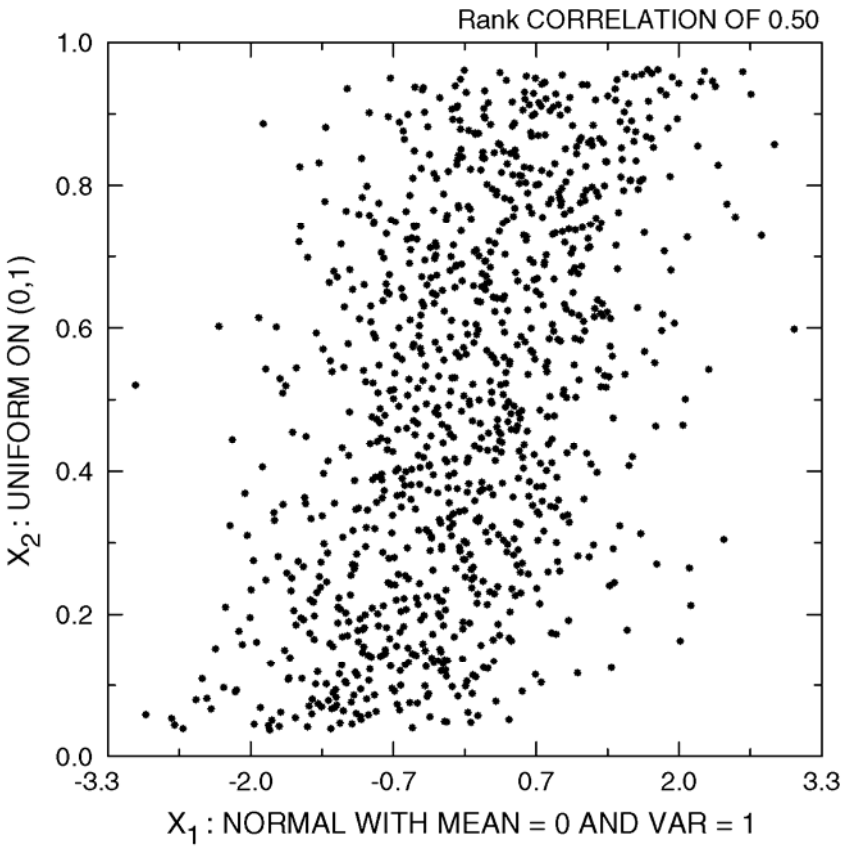
- Imposition of complex correlation structure not easy

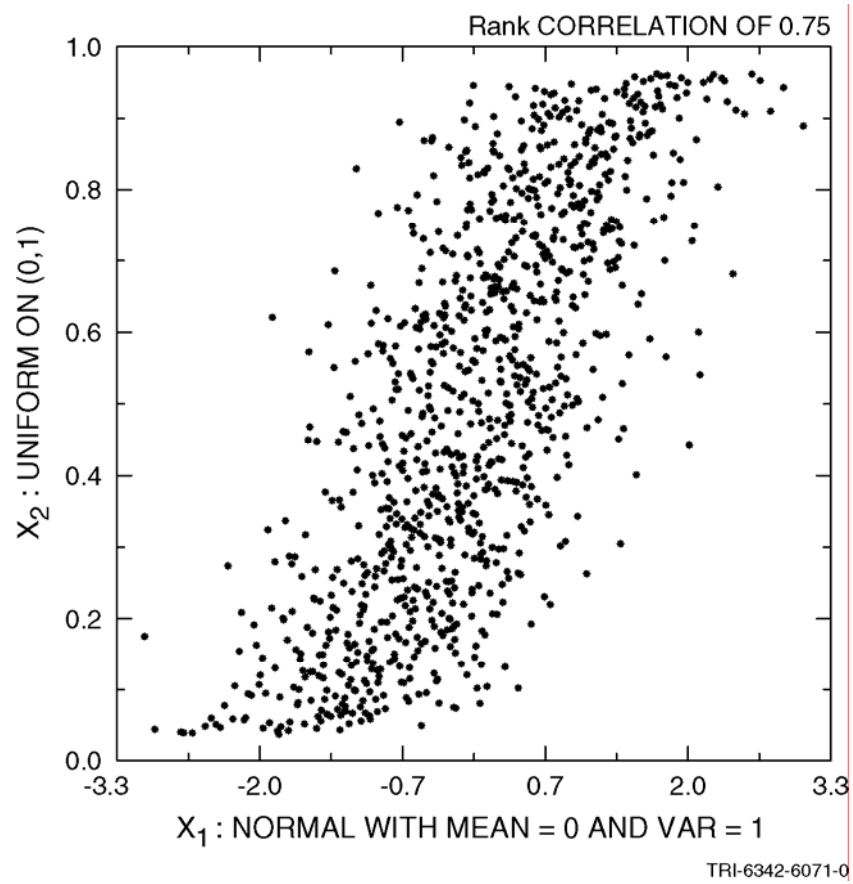
- Iman and Conover have developed method to impose rank correlations
  - Distribution free
  - Works with random and LH sampling
  - Preserves intervals used in LH sampling

Correlation Control: Example

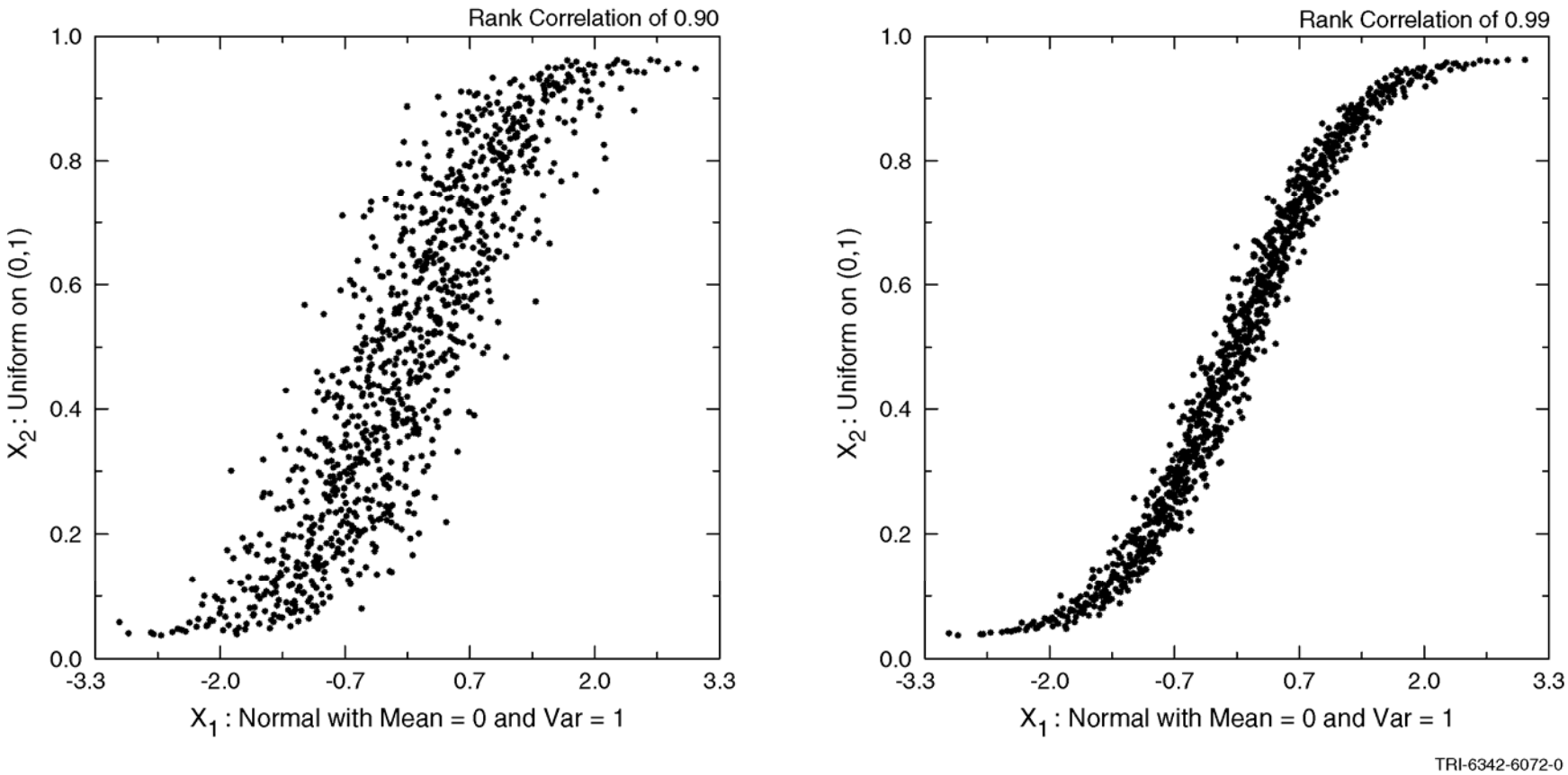


Correlation Control: Example (cont)





Correlation Control: Example (cont)



Example Analysis: Generation of Sample

- LH sampling used
- *nLHS* = 300 samples from *nX* = 31 variables
- Sample: $\boldsymbol{x}_k = [x_{1k}, x_{2k}, \ldots, x_{31,k}]$, $k = 1,2,\ldots,300$
- Tests for robustness
  - Sample generated as 3 independent replicated samples of size 100 each
  - Individual replicated samples

    R1: $\boldsymbol{x}_k$, $k = 1,2,\ldots,100$
    R2: $\boldsymbol{x}_k$, $k = 1,2,\ldots,100$
    R3: $\boldsymbol{x}_k$, $k = 1,2,\ldots,100$
- Iman/Conover technique used to control correlations

Propagation of Sample through Analysis

- Generates mapping $[\boldsymbol{x}_k, \boldsymbol{y}(\boldsymbol{x}_k)]$, $k = 1,2,\ldots,nS$

- Requires evaluation of $\boldsymbol{y}(\boldsymbol{x}_j)$
  - Details analysis specific
  - Can be most computationally demanding part of analysis

- Example analysis
  - Required 4-5 hrs CPU time per model evaluation on VAX Alpha
  - Produced large quantity of temporally and spatially variable results

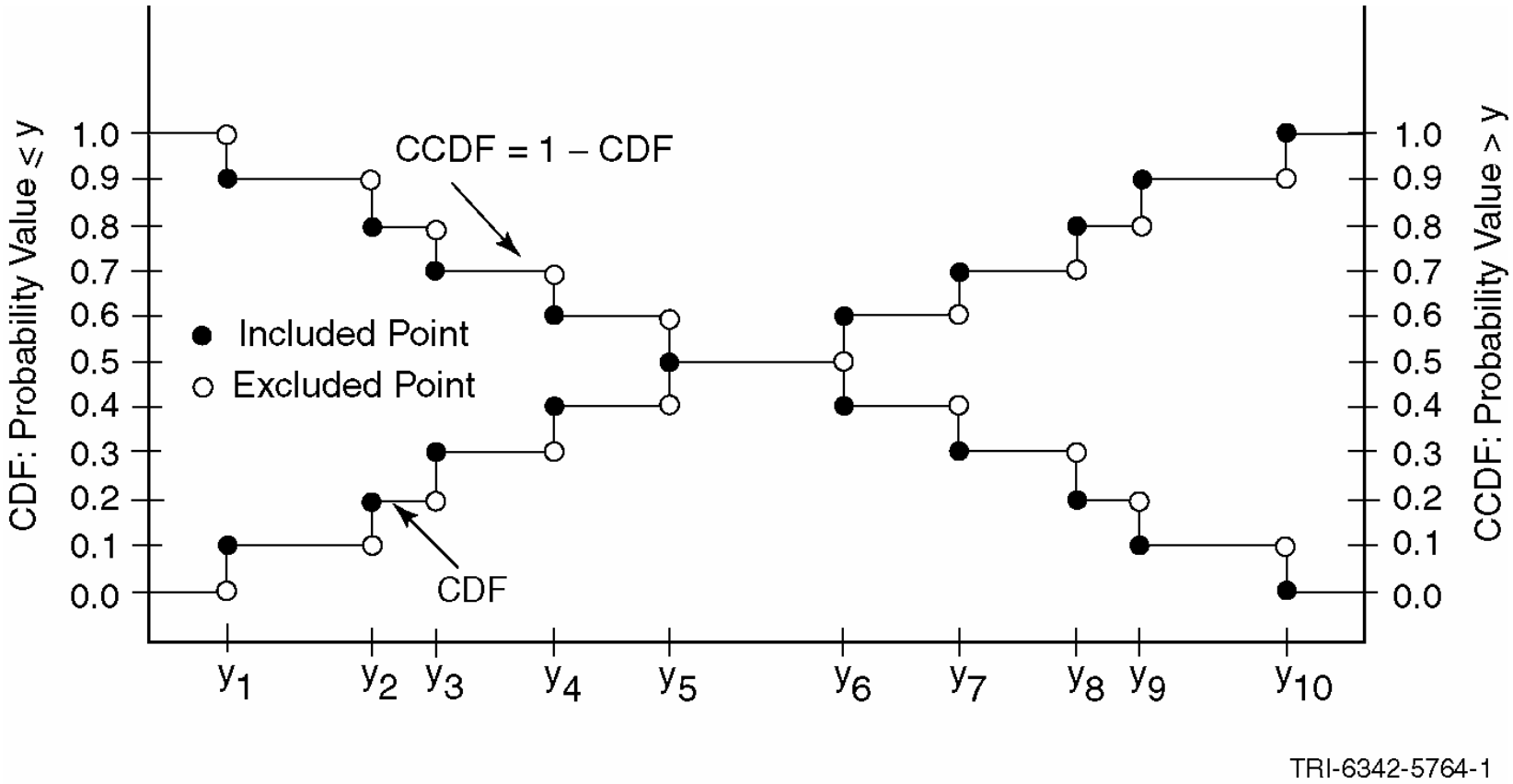
Uncertainty Analysis: Scalar Results

- Single scalar result: $y_k = y(\boldsymbol{x}_k)$, $k = 1,2,\ldots,nS$
- Mean and variance

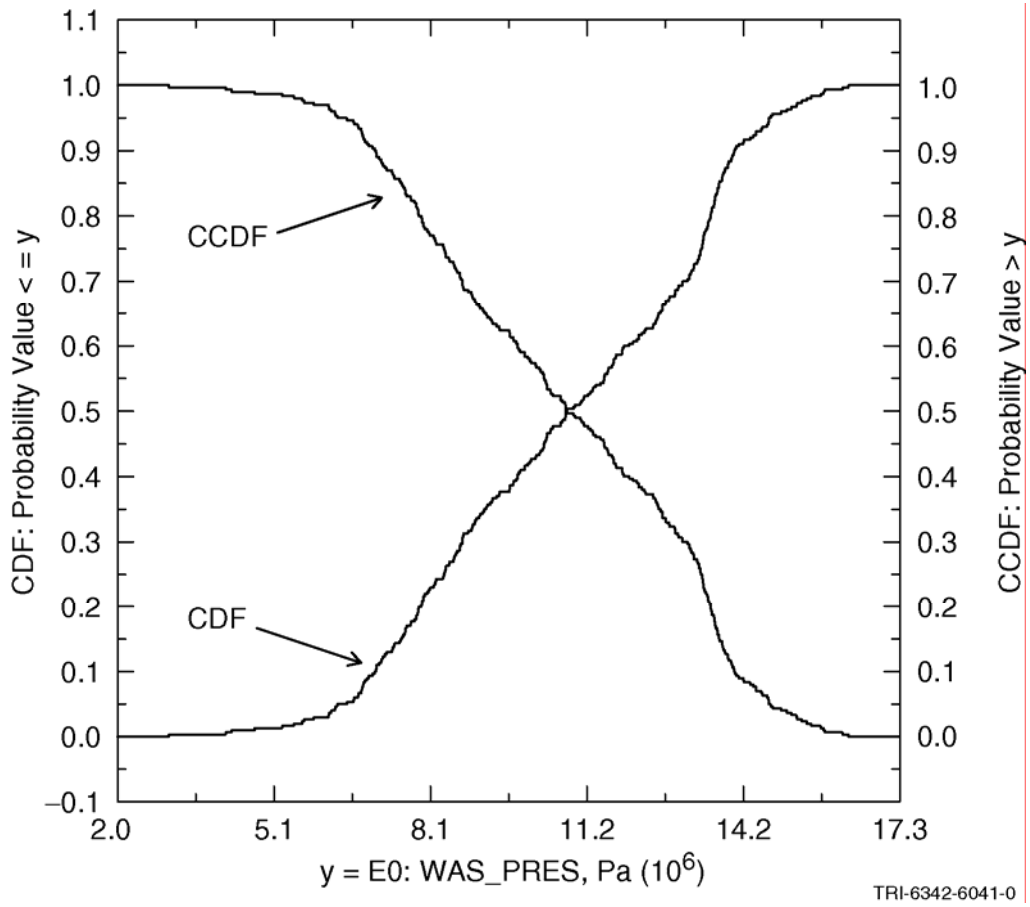
$$\hat{E}(y) = \sum_{k=1}^{nS} y_k \,/\, nS, \quad \hat{V}(y) = \sum_{k=1}^{nS} \left[y_k - \hat{E}(y) \right]^2 \Big/ (nS - 1)$$

Uncertainty Analysis: Scalar Results (cont)

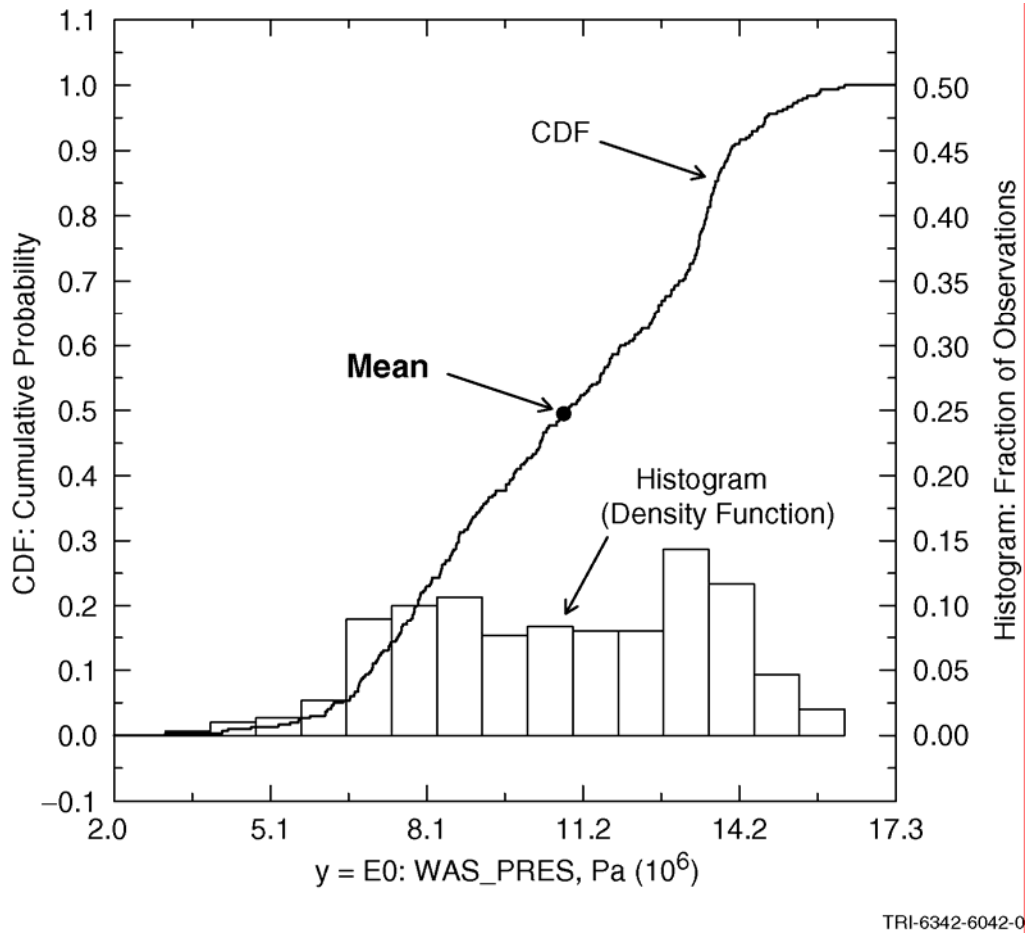
- Distribution function



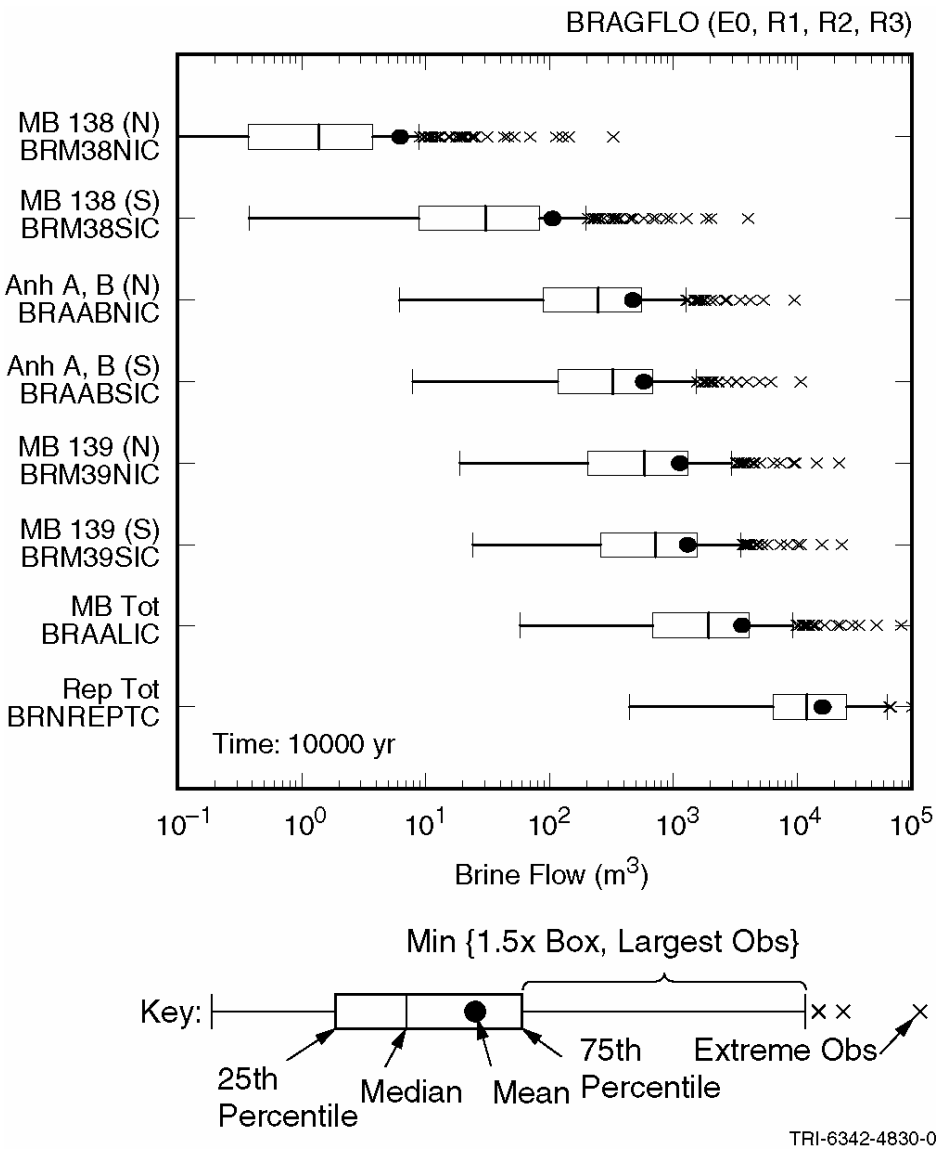
Example Analysis: CDFs and CCDFs



Example Analysis: CDF and Density Function

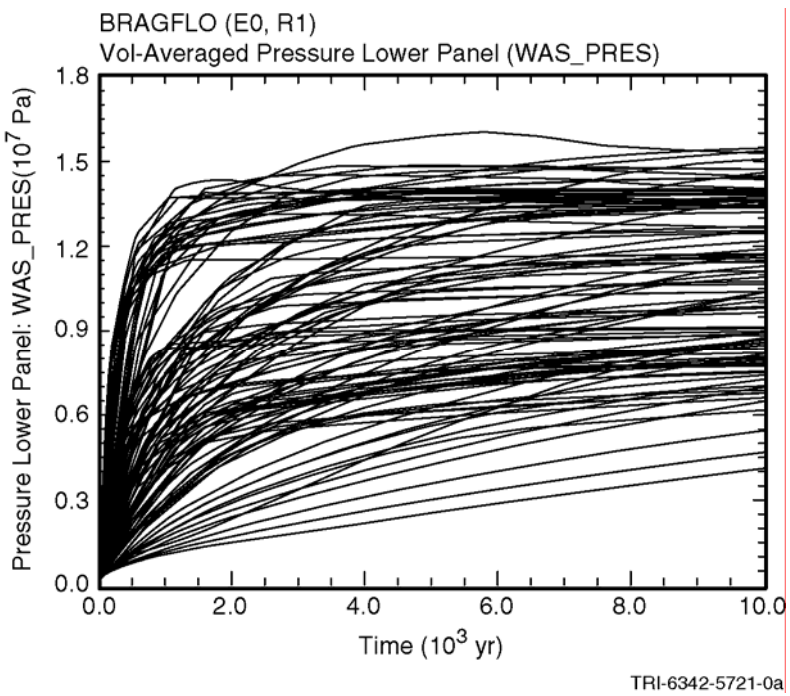


Example Analysis: Box Plots

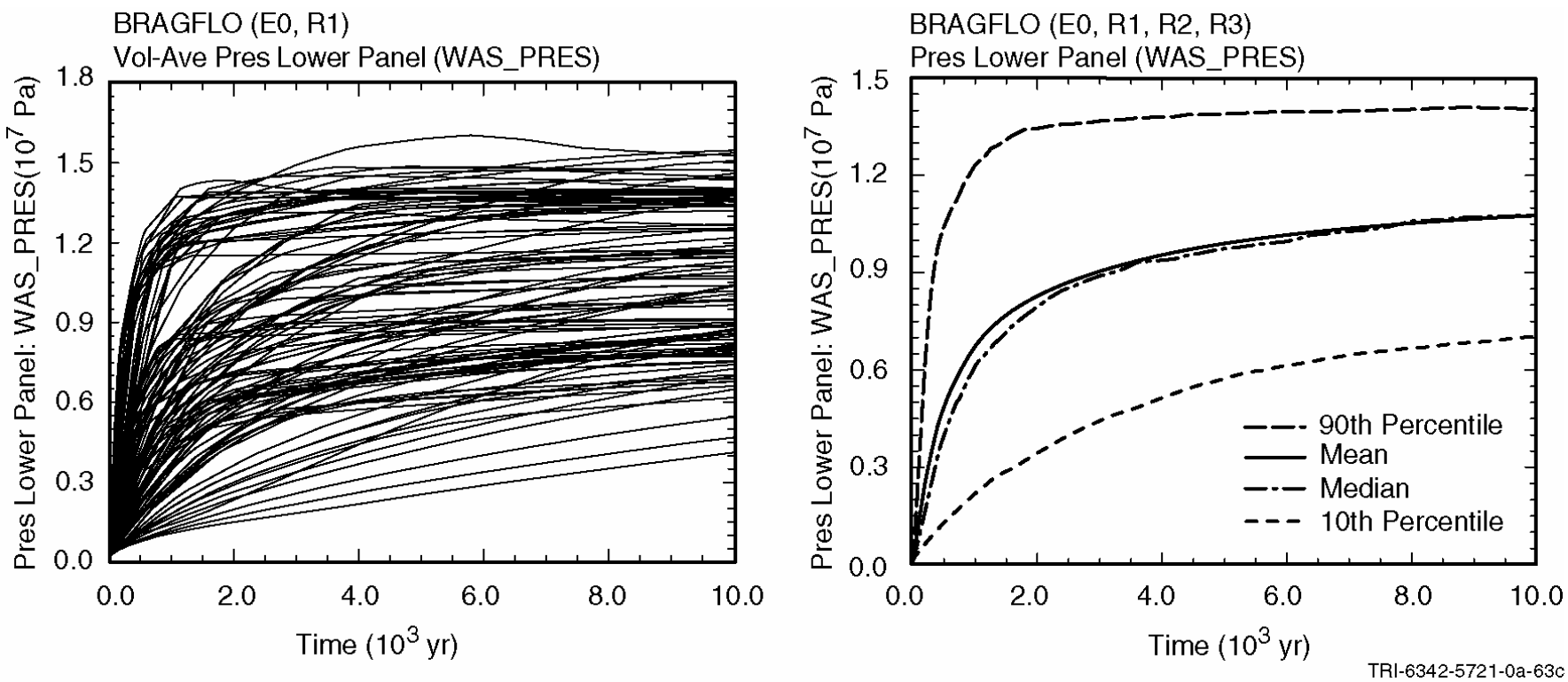


Uncertainty Analysis: Functions

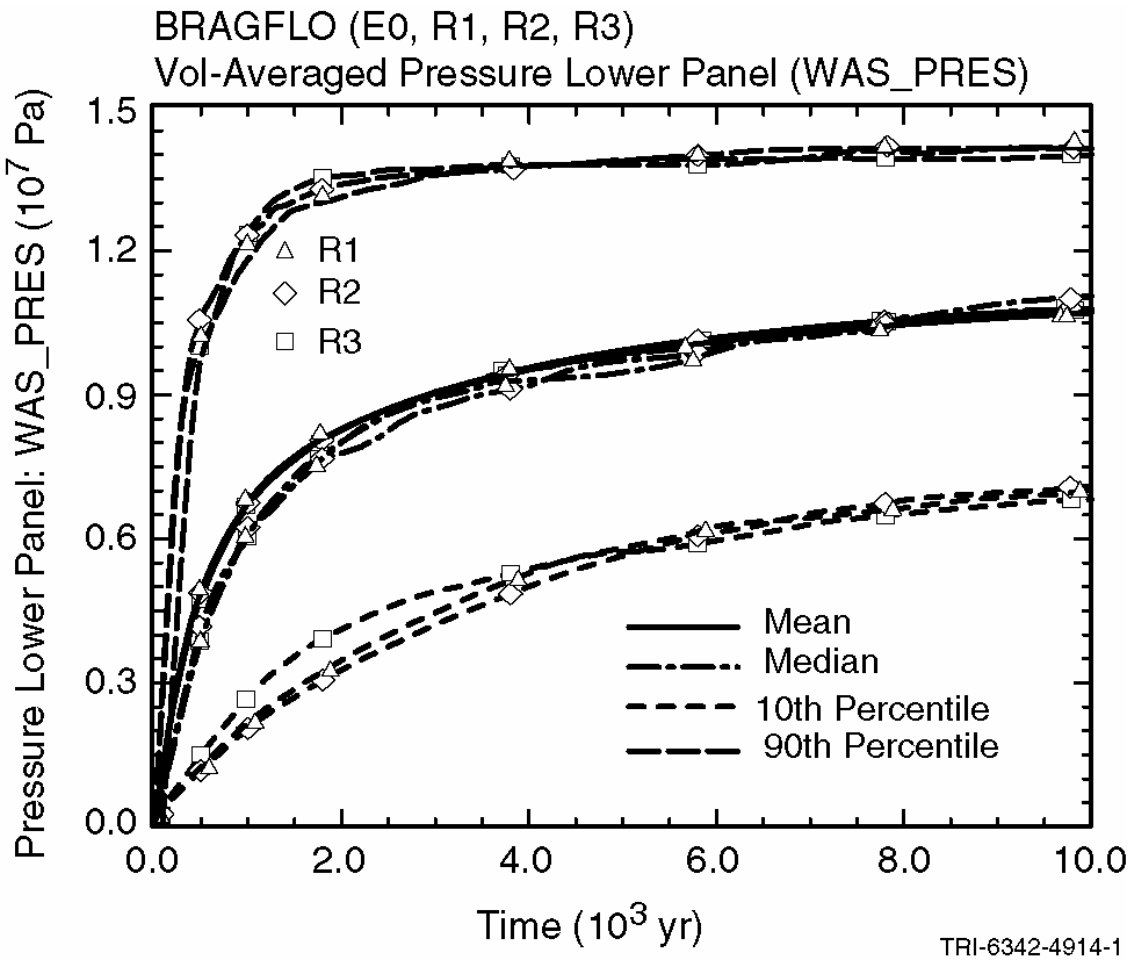
- Analysis outcomes are often functions of one or more variables
- Uncertain analysis inputs result in many possible values for such functions
- Example analysis: pressure as a function of time



Example Analysis: Pressure at Time *t*



Example Analysis: Replicated Samples and Stability



Sensitivity Analysis

- Involves exploration of mapping $[\boldsymbol{x}_k, \boldsymbol{y}(\boldsymbol{x}_k)]$, $k = 1,2,\ldots,nS$
- Available techniques for sensitivity analysis
  - Examination of scatterplots and cobweb plots
  - Correlation and partial correlation analysis
  - Regression analysis
  - Stepwise regression analysis
  - Rank transforms to linearize monotonic relationships
  - Nonparametric regression: Loess, additive models, projection pursuit, recursive partitioning
  - Tests for patterns based on gridding: nonmonotonic relations, nonlinear relations

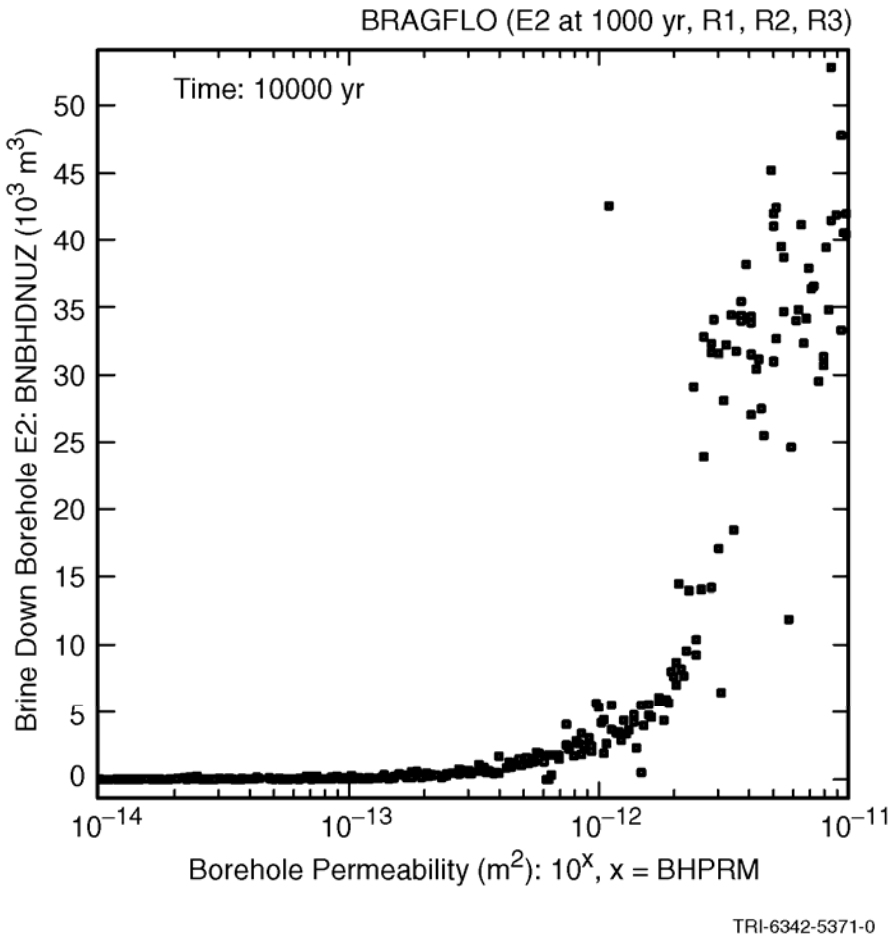
Sensitivity Analysis (Continued)

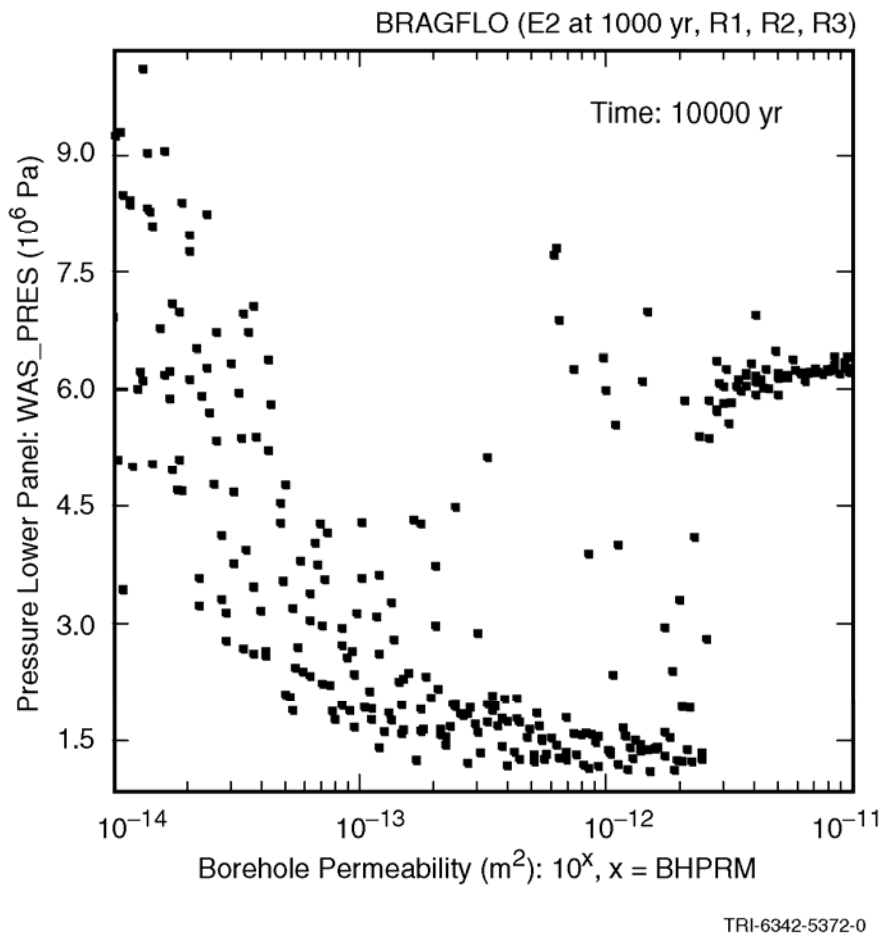
- Tests for patterns based on distance measures
- Multidimensional Kolmogorov-Smirnov test
- Tree-based searches
- Squared differences of ranks
- Top-down concordance with replicated samples
- Variance decomposition

Examination of Scatterplots

- Simplest sensitivity analysis technique
- Points (x_{jk}, y_k), $k = 1,2,\ldots,nS$, plotted for each x_j in $\boldsymbol{x}$
- Resulting plots visually examined for patterns
- Effective with LH sampling due to full stratification over range of each x_j
- Examples follow

Example Analysis: Scatterplots

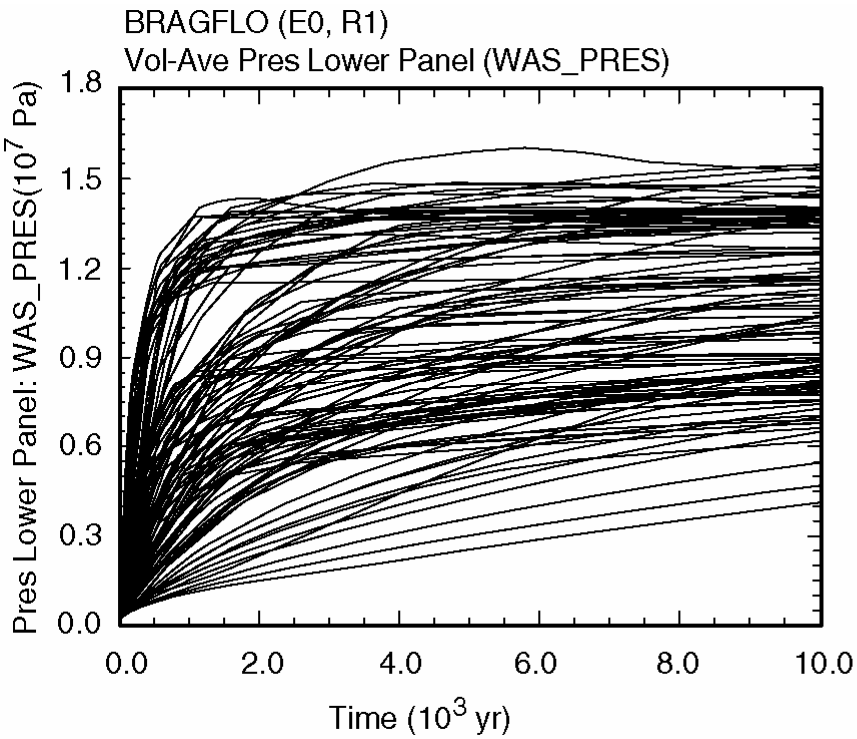


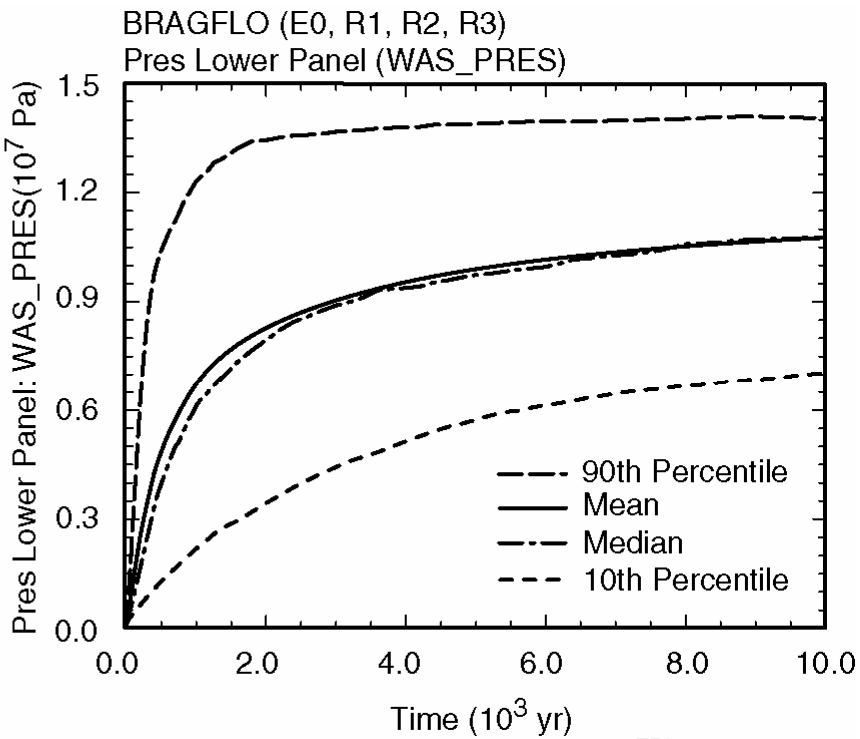


Stepwise Regression: Ranking Variable Importance

- Order of selection in stepwise procedure
- Changes in R^2 values at successive steps
- Absolute values of SRCs
- With independent sampled variables, three preceding ranking procedures produce same ordering of variable importance

Example Analysis: Pressure at Time *t*





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Example Analysis: Compact Representation of Stepwise Regression

- Compact Summary of Stepwise Regression Analyses for Pressure in the Repository at 10,000 yr Under Undisturbed Conditions (i.e., *y* = *E0:WAS_PRES* at 10,000 yr)

Step[a]	Variable[b]	SRC[c]	R^{2}[d]
1	*WMICDFLG*	0.718	0.508
2	*HALPOR*	0.466	0.732
3	*WGRCOR*	0.246	0.792
4	*ANHPRM*	0.129	0.809
5	*SHRGSSAT*	0.070	0.814
6	*SALPRES*	0.063	0.818

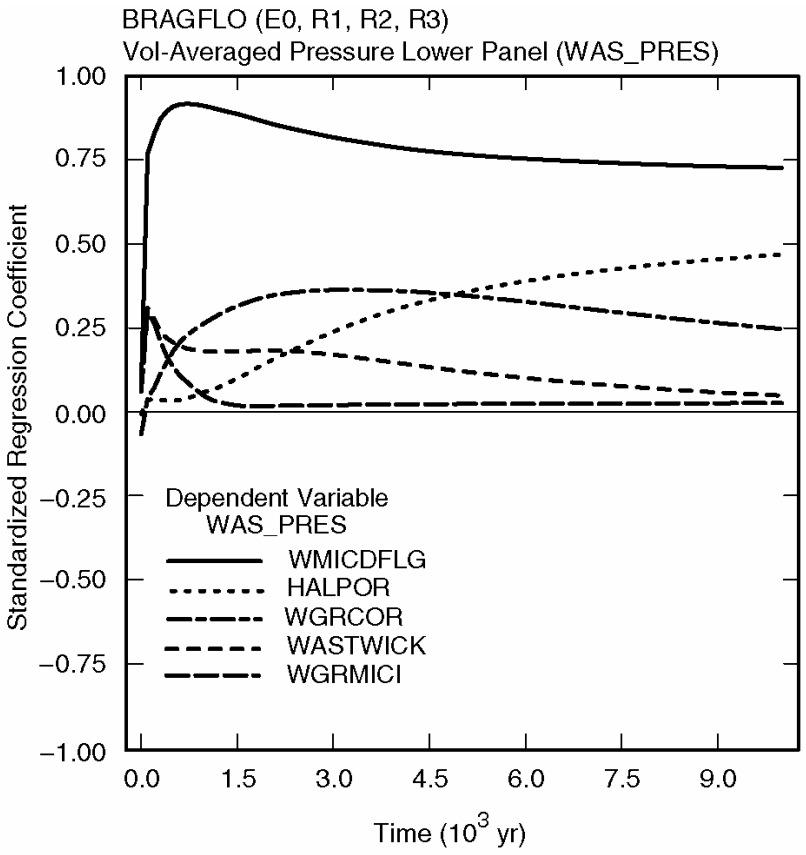
[a] Steps in stepwise analysis.

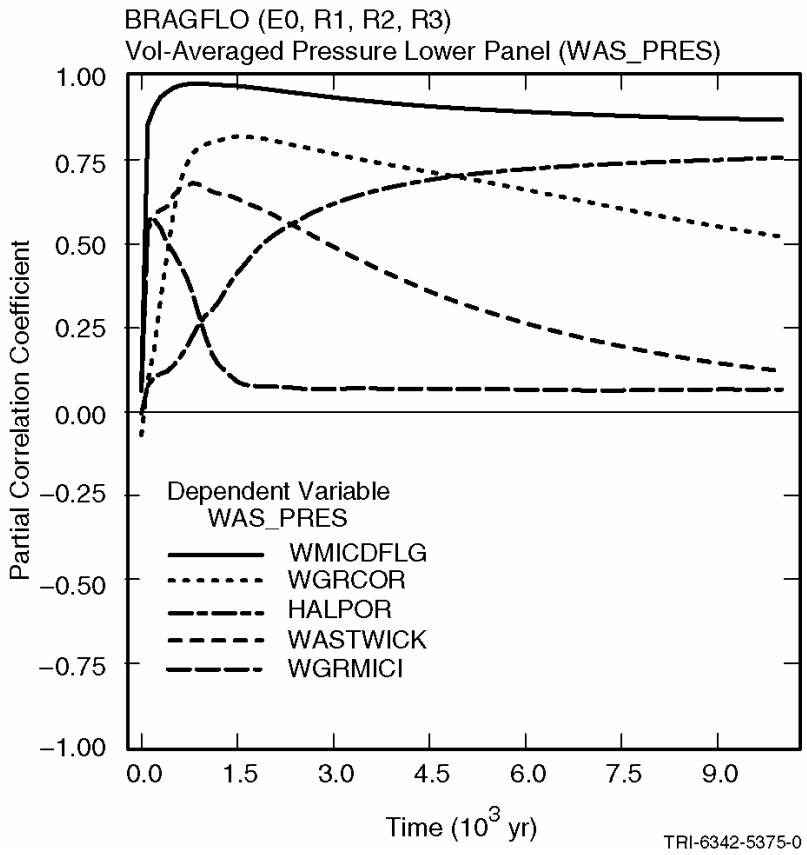
[b] Variables listed in the order of selection in regression analysis.

[c] Standardized regression coefficients (SRCs) for variables in final regression model.

[d] Cumulative R^2 value with entry of each variable into regression model.

Example Analysis: Time-Dependent SRCs and PCCs

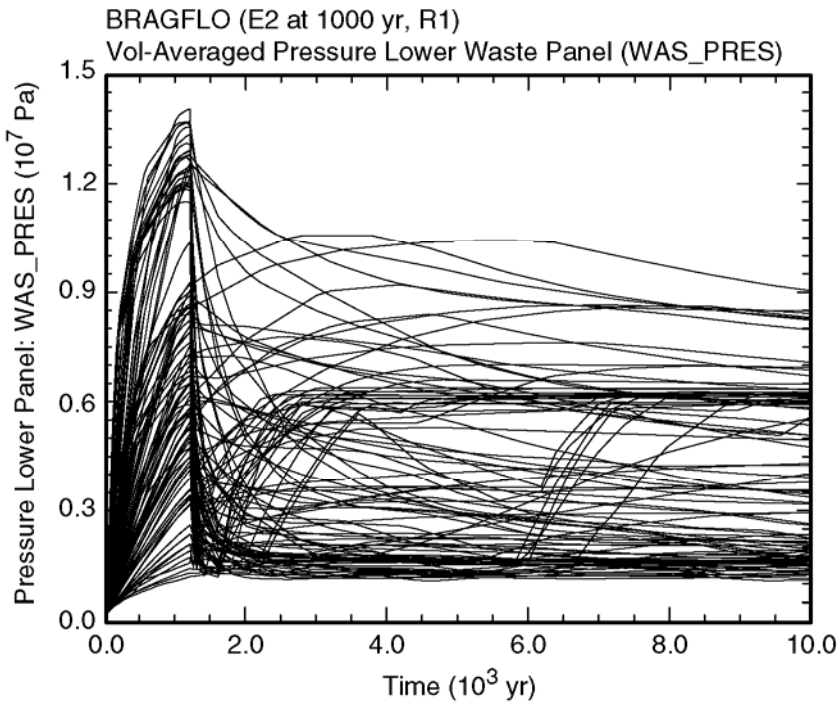


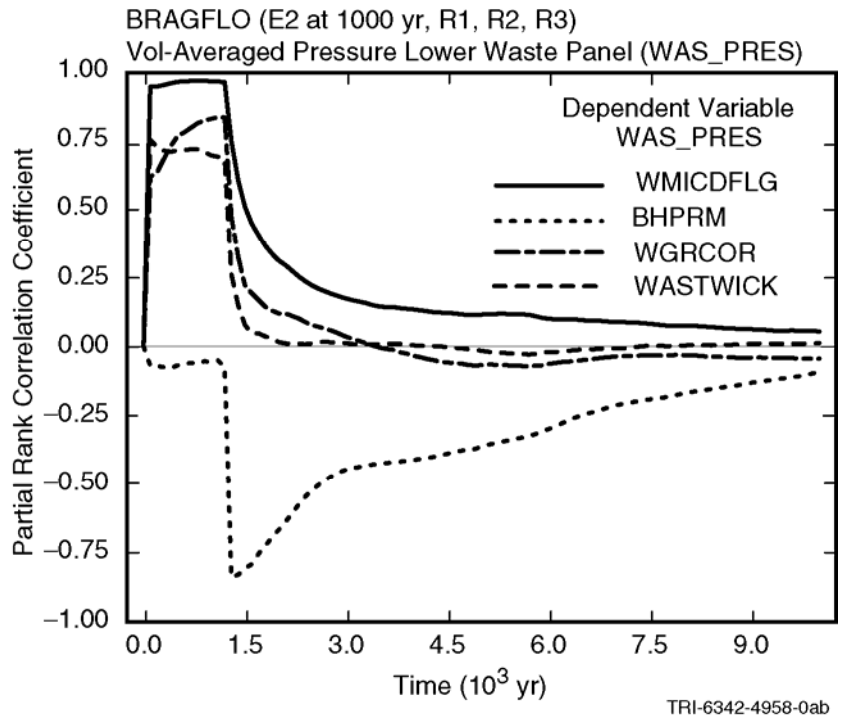


Identification of Nonmonotonic Patterns

- Regression-based sensitivity analyses sometimes perform poorly
- Rank transformations possible alternative
  - Linearizes monotonic relationships
  - Will not help for nonmonotonic relationships
- Example follows

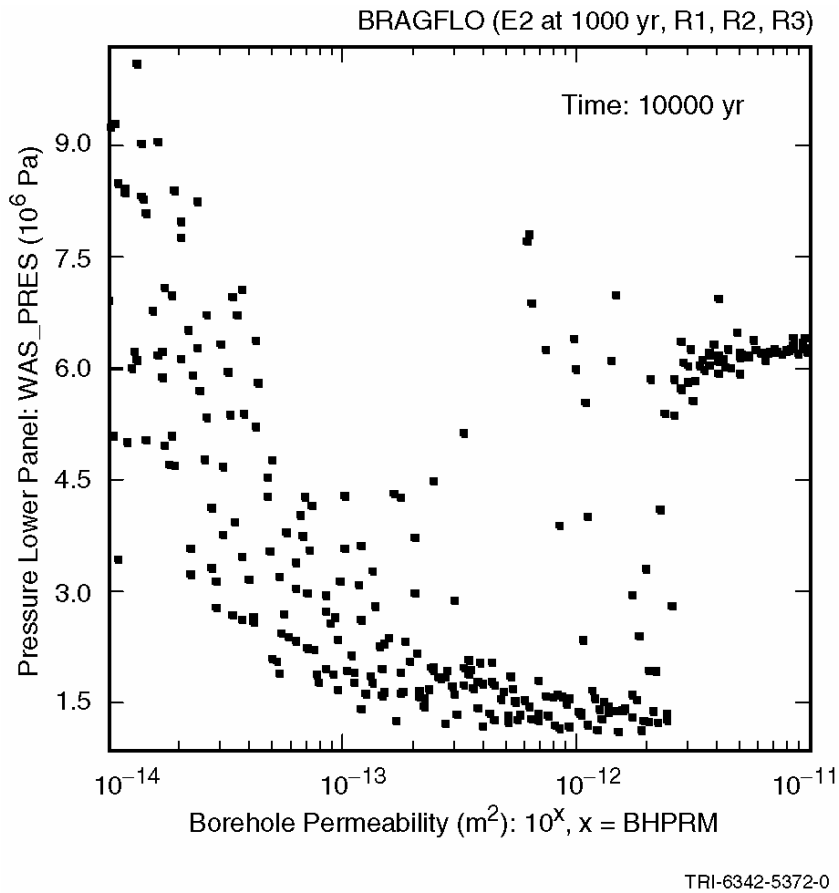
Example Analysis: Failure of Regression-Based Techniques





Example Analysis: Failure of Regression-Based Techniques (cont)

- Examination of scatterplots identified dominant variable

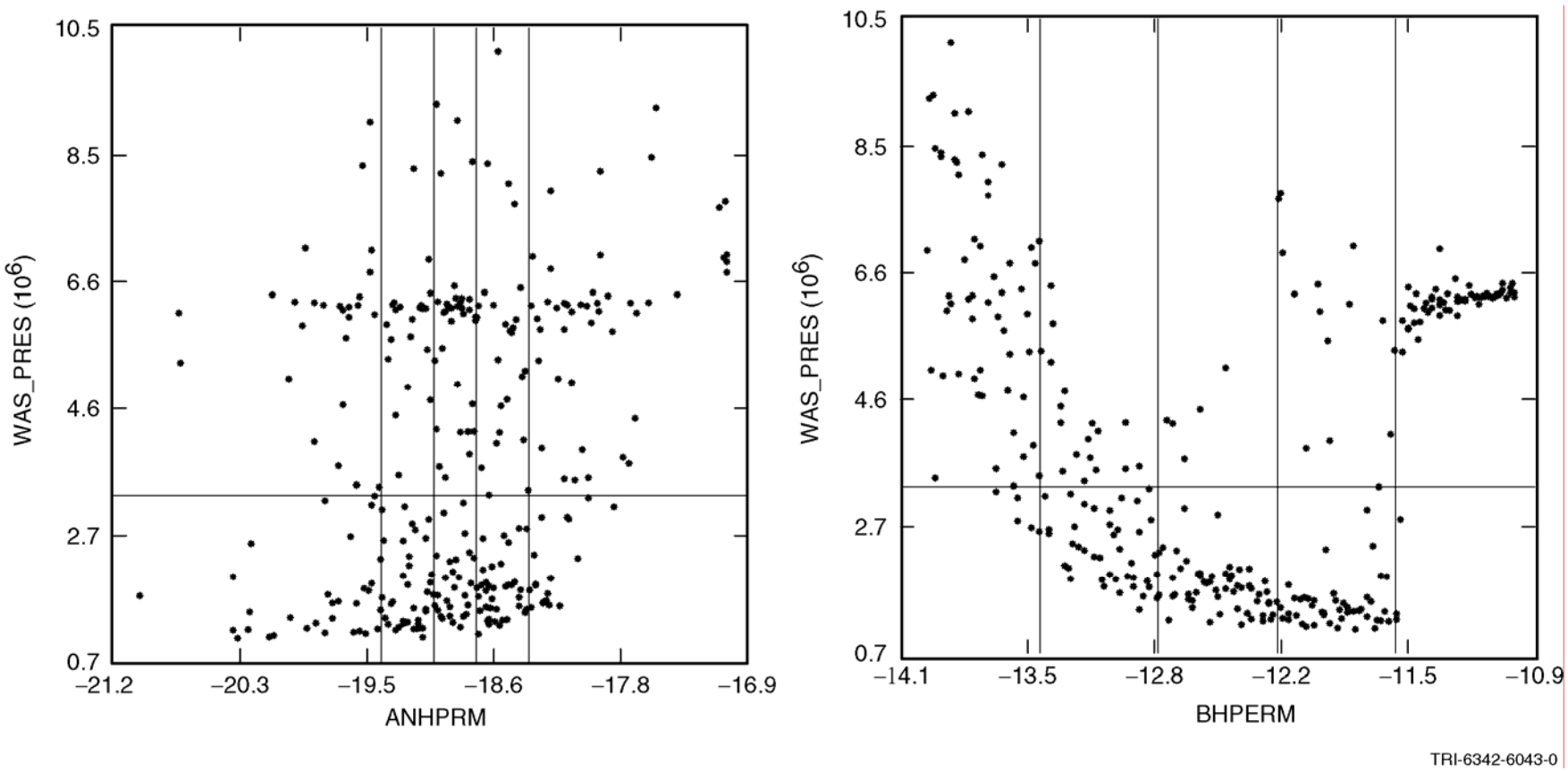


Test for Nonmonotonic Patterns

- Three tests
  - *F*-test for common means (CMNs)
  - χ^2-test for common medians (CMDs)
  - Kruskall-Wallis test for common locations (CLs)

- Tests based on
  - Subdividing values of x_j into intervals
  - Testing to determine if *y* has common measure of central tendency across these intervals

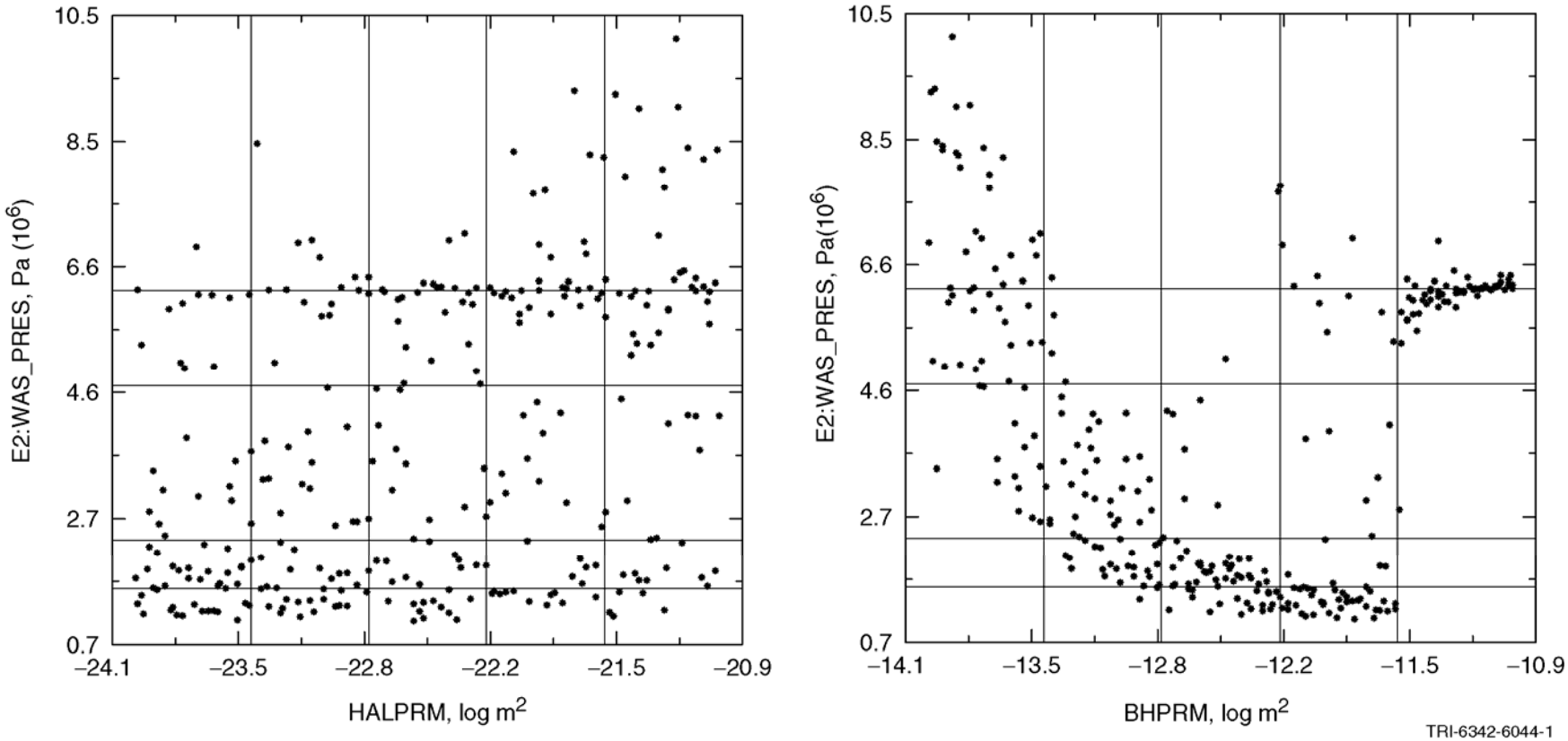
Tests for Nonmonotonic Patterns: Subdivision of x_j



Identification of Random Patterns

- Determine if points in scatterplot appear to be random conditional on distributions for x_j and y
- Based on dividing points into two-dimensional grid
- χ^2-test used to indicate if scatterplot appears to be random
- Denoted test for statistical independence (SI)

Identification of Random Patterns: Subdivision of x_j, y



Additional Information

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