VALIDATION OF MULTIVARIATE MONTE CARLO STUDIES.

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OUTLINE:

* Introduction and Background
  - Factors and Requirements.

* Planning Stage Activities
  - Generation of Multivariate Alternatives

* Concurrent Stage Activities
  Following the Validation Roadmap

* Final Stage Activities
  - Using the Final Results

* Conclusions
I. INTRODUCTION AND BACKGROUND:

* Validation (monitoring): a necessary evil

- Factors Fostering M.C. studies: computer development
  - Uses: Proving/Developing New Statistical Methods

* Validation (as opposed to Verification)

* Monte Carlo (as opposed to System Simulation)

  - Less Opportunities for Validation Activity
    - No Real System to Compare With
    - No Output Analysis Stream
    - The Statistical Model is It

* Multivariate (as opposed to Univariate)

  - Many More Parameters to Control
  - More Difficult Transformations to Perform
    - Unknown Resulting Distributions
    - Dimensionally, Difficult to Imagine

* This Paper: Three-Phase Validation Scheme

  - Planning, Concurrent and Final Stages

* Objective: Convert Validation from Nuisance to QC Tool
* Example of Large Scale M.C. Study:

  - Objective: Power/Comparison Study
  - New Methods: Two; Established Methods: Eight
  - Sample sizes: Four; Number of p-variates: Seven
    - Correlation Structures: Two
  - Statistical Distributions: Twelve; Settings: Two
    - Total Experimental Runs: Three Hundred.

II. PLANNING STAGE ACTIVITIES:

* At Onset of the Study

  - Jointly With General Design Stage
    - Include in Literature Search
  - Seek: previous studies and asymptotic/special cases

* Examples in Previous Studies:

  - Partial results: Mardia, Koziol, some e.c.v.
  - Asymptotic Theory: Mardia Koziol test distribution
  - Special Cases: Laplace for the K-Distribution
    - Use as Initial Validation Parameters

* Generation of Multivariate Distributed Alternatives

  - General Problems: performance/robustness
  - General Factors: sample, variates, correlation, shape
    - Distributions: Study Problems of Shape
* Distribution Classification by Shape

- Cross Validation Schemes in Classification by Shape

* A Classification of Multivariate Generation Approaches

* 1. "Indirect": Generation

* Combining Natural Univariate Distributions

  - Use Correlation Structure Desired
  - Resulting Distribution Unknown
  - Little Control on Resulting Skew/Kurt
    - Easy to Implement
  - Examples of Natural Univariate Distributions

* Combining Empirical Univariate Families

  - GDL, Johnson and Pearson Families
  - Easy to Generate, Variety of Shapes, Larger Control
    - Restricted Domain (Artificial)
    - Mixture of Multivariate Normals
    - Covariance Structure Obtained
    - Little Distribution Information
      - Bottom/up Approach
      - Skewness Problems
  - Use Graphical Bivariate Information
2. "Direct" Generation

* Conditional Distribution Approach
  - Derivation of Marginal/Conditional Distr.
  - Not Always Feasible/Convenient
    - Top/Down Approach

* Transformation Approach
  - Not Always Feasible/Convenient to Find
    - Also Top/Down
  - Most Used in Multivariate Normal Generation
  - Johnson’s Multivariate Transformation System
  - Johnson’s Bivariate Theoretical/Graphical Study
  - Study/Compare Nomograms for Johnson/Mixtures
    - Use Graphs/Nomograms as Validation Tools
  - Select Alternatives as per Study Requirements
    - Bottom/Up Approach

3. "Factorization" Approach

* Elliptically Contoured/Spherically Sym. Distributions
  - Obtaining the Multivariate Vector
    - The Univariate "Driver"
  - Examples: Multivariate Pearson II and VII
    - Another "Factorization" Scheme
  - Obtaining the Multivariate Vector
- The Univariate Driver
- Comparison of Both Approaches
- Example: Validation of the K-Distribution (Laplace)

* Random Number Generators

- Careful About Packaged Software
- Generation of the Uniform Vector in the Hypersphere

* Summarization of Initial Stage:

- Where Validation Parameters Are Defined
- Where Validation Roadmap is Drafted

III. CONCURRENT STAGE

* All Along the M.C. Study
  * Use as a QC. Tool
  * Verify Every Validation Parameter Defined
  * Check Any Package Software Used
  * Check Incomming Results With Previous Studies
  * Check Results Under the Null (Testing for \( \alpha \))
  * Use Graphical Validation (Bivariate Case)
* Obtain/Check Large Sample Estimators of Your Parameters
* Cross Validate Using Different Schemes (Mardia's Plot)
  * Perform Sensitivity Analyses (use \( \rho \))
* Compare/Test Similar Methods of Generating r.v.
  * Document Results Carefully
We say (and denote) \( X \sim EC_p(\mu, \Sigma; g) \) if its density:

\[
f(x) = \kappa_p |\Sigma|^{-1/2} g((X_i - \mu)' \Sigma^{-1}(X_i - \mu))
\]

where \( \kappa_p \) is a normalizing constant and \( g(.) \) a continuous variable.

Therefore, \( X \) can be generated by multiplying \( R \) by \( U^{(p)} \):

\[
X = R \Sigma^{1/2} U^{(p)} + \mu
\]

where \( R \) is a positive random variable, independent of \( U^{(p)} \), having the distribution of \( \sqrt{(X_i - \mu)' \Sigma^{-1}(X_i - \mu)} \). And \( B \) is a \( p \times p \) matrix such that \( BB' = \Sigma \).

The univariate \( R^2 \) has density:

\[
h(z) = \frac{\pi^{p/2}}{\Gamma(p/2)} \kappa_p z^{p/2-1} g(z)
\]

where \( z = (X - \mu)' \Sigma^{-1}(X - \mu) \).

For the multivariate normal (p), \( R^2 \) is the \( \chi^2_p \) and \( \kappa_p = (2\pi)^{-p/2} \) and \( g \) the identity. For the Pearson Type II, \( R^2 \) is \( Beta(p/2, m + 1) \). And for Pearson Type VII, \( R^2 \) is the univariate Pearson Type VI. This last type is generated via:

\[
R^2 = Y/(1 - Y), \quad \text{where} \quad Y \sim Beta(p/2, m - 1/2)
\]

The density function of the p-dimensional Pearson II distribution is:

\[
f(x) = \frac{\Gamma(\frac{m}{2} + m + 1)}{\Gamma(m + 1)\pi^{p/2}} |\Sigma|^{-\frac{1}{2}} \left\{1 - (X_i - \mu)' \Sigma^{-1}(X_i - \mu)\right\}^m
\]

Its marginals are also Pearson type II distribution, with kurtosis:

\[
\frac{3(m + \frac{p}{2} + 1)}{m + \frac{p}{2} + 2} \rightarrow 3 \quad \text{as} \quad m, p \rightarrow \infty
\]

The density function for the p-dimensional Pearson type \( \text{VII} \) is:

\[
f(x) = \frac{\Gamma(m)}{\Gamma(m - \frac{p}{2})} |\Sigma|^{-\frac{1}{2}} \left\{1 + (X_i - \mu)' \Sigma^{-1}(X_i - \mu)\right\}^{-m}
\]

A more recent approach to this problem is that of Rangaswamy, Weiner and Ozturk (1992). They decompose the multivariate \( X \sim \mathcal{F} \) using the factorization \( X = SZ \). Here, \( Z \sim \mathcal{MN}_p(0, \Sigma) \) and \( S \) is a univariate r.v. driving the multivariate distribution of \( X \) such that:

\[
f_X(X) = (2\pi)^{-p/2} |M|^{-1/2} h_p(q); \quad \text{where} \quad q = X'M^{-1}X
\]

where \( h_p(q) = \int_0^\infty s^{-p} \exp\left(-\frac{q}{2s^2}\right) f_S(s) \, ds \) and \( \Sigma = ME(S^2) \).
Table 3: Regressions of ecv on Sample Sizes.

<table>
<thead>
<tr>
<th>ROW</th>
<th>p</th>
<th>eta</th>
<th>ecv</th>
<th>C.V.</th>
<th>sigma</th>
<th>IoF</th>
<th>MVN GOF Test:</th>
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<td>1</td>
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<td>0.90</td>
<td>7.790</td>
<td>7.78</td>
<td>0.027</td>
<td>0.99</td>
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</tr>
<tr>
<td>3</td>
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<td>0.065</td>
<td>0.98</td>
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</tr>
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</table>
| 4   | 2  | 0.90| 4.580| 4.61 | 0.014 | 0.98| Cox and Small
| 5   | 2  | 0.95| 5.990| 5.99 | 0.032 | 0.94| "               |
| 6   | 2  | 0.99| 9.100| 9.21 | 0.078 | 0.94| "               |
| 7   | 2  | 0.90| 0.989| *    | 5.500& | 0.99| Malkovich-Afifi|
| 8   | 2  | 0.95| 0.989| *    | 5.800& | 0.99| "               |
| 9   | 2  | 0.99| 0.989| *    | 7.500& | 0.99| "               |
| 10  | 2  | 0.90| 1.630| 1.65 | 0.012 | 0.99| Mardia Kurt.(LB)|
| 11  | 2  | 0.95| 2.080| 1.95 | 0.016 | 0.99| "               |
| 12  | 2  | 0.99| 2.900| 2.58 | 0.036 | 0.92| "               |
| 13  | 2  | 0.90| -1.550| -1.65| 0.011 | 0.96| "               |
| 14  | 2  | 0.95| -1.770| -1.95| 0.018 | 0.95| "               |
| 15  | 2  | 0.99| -2.180| -2.58| 0.032 | 0.93| "               |
| 16  | 2  | 0.90| 1.060| *    | 5.200& | 0.14@| Hawkins         |
| 17  | 2  | 0.95| 1.320| *    | 7.700& | 0.04@| "               |
| 18  | 2  | 0.99| 1.940| *    | 1.500& | 0.08@| "               |
| 19  | 2  | 0.90| 4.630| 4.61 | 0.037 | 0.30@| Koziol Angles  |
| 20  | 2  | 0.95| 5.990| 5.99 | 0.060 | 0.11@| "               |
| 21  | 2  | 0.99| 9.110| 9.21 | 0.157 | 0.04@| "               |

* Empirical tests; no asymptotic distribution available.

@ Critical Value was independent of sample size.

& Exponential notation; four decimal places (i.e 5.5*10^-4).
Table 4: 95% Nonparametric Confidence Intervals.

<table>
<thead>
<tr>
<th>ROW</th>
<th>p</th>
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<th>eta</th>
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</tr>
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<td>Cox and Small</td>
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<tr>
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<td>15.51</td>
<td>18.25</td>
<td>19.530</td>
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</tr>
</tbody>
</table>

* Rho is the p-variate correlation coefficient.

* ecv's LB (confidence interval lower bounds) and UB (upper bounds) were empirically obtained with 10,000 replications for p=2 and with 5,000 replications for p>2.

* CV is the asymptotic critical value, for the corresponding percentile, (eta), of 90, 95, 98 or 99 percent for the test in question.
IV. FINAL STAGE

* After the Final Results Are IN.
* Dependent on the M.C. Objectives
* Use the Asymptotic and/or Special Cases Found
* Example w/Asymptotic Values: Regression on size
* Example w/Asymptotic Values: Confidence Intervals
  * Example w/Special Case: Laplace Distribution

V. CONCLUSIONS

* Validation: Time Consuming and Complex
  * All Results Depend on this Activity
  * Implement as a QC. Research Tool
    * Use Generation Procedures
    * Use Data From Previous Studies
      * Use Asymptotic/Special Cases

* APPLIED STATISTICS GRADUATE COURSE

***
Refs


