VALIDATION OF MULTIVARIATE

MONTE CARLO STUDIES.

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OUTLINE:

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*** 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 Controured/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**

- *Carefull 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 α)**

*** 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 ρ)**

*** Compare/Test Similar Methods of Generating r.v.**

*** Document Results Carefully**

We say (and denote) $\mathbf{X} \sim EC_p(\mu, \Sigma; g)$ if its density:

$$f(x) = \kappa_p |\Sigma|^{-1/2} g((\mathbf{X}_i - \mu)'\Sigma^{-1}(\mathbf{X}_i - \mu))$$

where κ_p is a normalizing constant and $g(.)$ a continous variable.

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

$$\mathbf{X} = RBU^{(p)} + \mu$$

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

The univariate R^2 has density:

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

$$where \quad z = (\mathbf{X} - \mu)'\Sigma^{-1}(\mathbf{X} - \mu)$$

For the multivariate normal (p), R^2 is the χ^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:

$$R^2 = Y/(1-Y), \qquad where \qquad Y \sim Beta(p/2, m - 1/2)$$

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

$$f(x) = \frac{\Gamma(\frac{p}{2} + m + 1)}{\Gamma(m+1)\pi^{\frac{p}{2}}} |\Sigma|^{-\frac{1}{2}} \{1 - (\mathbf{X}_i - \mu)'\Sigma^{-1}(\mathbf{X}_i - \mu)\}^m$$

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

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

The density function for the p-dimensional Pearson type VII is:

$$f(x) = \frac{\Gamma(m)}{\Gamma(m - \frac{p}{2})} |\Sigma|^{-\frac{1}{2}} \{1 + (\mathbf{X}_i - \mu)'\Sigma^{-1}(\mathbf{X}_i - \mu)\}^{-m}$$

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

$$f_{\mathbf{X}}(X) = (2\pi)^{-p/2} |M|^{-1/2} h_p(q); \qquad where \quad q = \mathbf{X}'M^{-1}\mathbf{X}$$

$$where \qquad h_p(q) = \int_0^\infty s^{-p} exp(\frac{-q}{2s^2}) f_S(s) ds \quad and \quad \Sigma = M\mathcal{E}(S^2)$$

Table 3: Regressions of ecv on Sample Sizes.

ROW	p	eta	ecv	C.V.	sigma	IoF	MVN GOF Test:
1	2	0.90	7.790	7.78	0.027	0.99	Mardia Skew.
2	2	0.95	9.670	9.49	0.044	0.98	" "
3	2	0.99	13.770	13.28	0.065	0.98	" "
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	" " (UB)
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*e-4).

Table 4: 95% Nonparametric Confidence Intervals.

ROW	p	rho	eta	CV	LB	UB	MVN GOF Test:
1	2	0.5	0.95	9.49	9.17	9.660	Mardia's Skew.
2	2	0.5	0.90	1.65	1.52	1.610	" Kurt.
3	2	0.5	0.95	5.99	6.11	6.533	Royston
4	2	0.5	0.95	5.99	5.94	6.290	Cox and Small
5	2	0.5	0.95	5.99	5.85	6.110	Koziol Angles
6	2	0.9	0.95	9.49	9.11	9.590	Mardia's Skew.
7	2	0.9	0.90	1.65	1.48	1.570	" Kurt.
8	2	0.9	0.95	4.61	4.78	5.070	Royston
9	2	0.9	0.95	5.99	5.85	6.230	Cox and Small
10	2	0.9	0.95	5.99	5.86	6.220	Koziol Angles
11	5	0.5	0.95	49.80	48.32	49.710	Mardia's Skew.
12	5	0.5	0.90	1.65	1.23	1.340	" Kurt.
13	5	0.5	0.95	11.07	10.83	11.410	Royston
14	5	0.5	0.95	11.07	20.05	26.990	Koziol Angles
15	5	0.9	0.95	49.80	48.43	49.760	Mardia's Skew.
16	5	0.9	0.90	1.65	1.27	1.410	" Kurt.
17	5	0.9	0.95	5.33	8.24	8.800	Royston
18	5	0.9	0.95	11.07	18.97	22.920	Koziol Angles
19	5	0.5	0.99	57.34	56.41	58.920	Mardia's Skew.
20	5	0.5	0.98	2.05	2.02	2.300	" Kurt.
21	8	0.5	0.95	145.98	143.32	145.610	" Skew.
22	8	0.5	0.90	1.65	1.08	1.190	" Kurt.
23	8	0.5	0.95	15.51	13.53	14.480	Royston
24	8	0.5	0.95	15.51	16.25	17.090	Koziol Angles
25	8	0.9	0.95	145.98	142.14	144.750	Mardia's Skew.
26	8	0.9	0.90	1.65	1.06	1.200	" Kurt.
27	8	0.9	0.95	5.55	9.12	9.660	Royston
28	8	0.9	0.95	15.51	18.25	19.530	Koziol Angles

* 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: Conficence 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

* * *

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