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**DISTRIBUTION FITTING WITH RESPONSE MODELING
METHODOLOGY- SOME RECENT RESULTS**

by

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ABSTRACT

Response Modeling Methodology (RMM) is a new approach for empirical modeling of systematic variation and random variation. While the former type of modeling results in an estimated non-linear relational model, the latter type yields an estimated quantile function that expresses quantiles of the data-generating distribution in terms of corresponding standard normal quantiles. Since its inception in the first years of the new millennium, RMM has been applied to various fields of science, engineering and operations management, and has been shown to deliver good modeling capabilities, while preserving desirable “uniformity of practice” across widely divergent disciplines. In this paper, RMM is briefly delineated, and its basic philosophy, relative to existent alternative approaches, is discussed. Recent modeling efforts that have used RMM to derive models for temperature-dependent chemical properties are briefly surveyed. Initial results from an ongoing PhD research that compares several families of distributions in terms of their capability to deliver good representation to commonly used statistical distributions are expounded. These results suggest that for families of distributions, commonly used for distribution fitting, like Pearson, generalized lambda, Burr and, more recently, RMM, ranking is feasible in terms of the associated values of the L_2 norm (a measure commonly used to assess goodness-of-fit).

1. INTRODUCTION

Response Modeling Methodology (RMM) is a new approach for empirical modeling of systematic variation and of random variation. Since its inception in the first years of the new millennium, RMM has been shown to include, as special cases, many models that have been derived independently within various scientific and engineering disciplines like physics, chemistry, chemical engineering, operations management and quality and reliability engineering. Furthermore, the error distribution of RMM has been shown to include as special cases various distributions, transformations and approximations, like the Johnson family of distributions, the Cauchy distribution, Tukey's g- and h- distributions and the inverse of the Box-Cox transformation (Shore, 2005, and references therein).

In this paper RMM is first briefly delineated (Section 2) and its core group of equations is introduced. We then expound (Section 3) the basic motivation that has triggered the development of RMM, and describe various problems, of essentially non-technical nature, that we believe exist with the current arsenal of methodologies for empirical modeling. How RMM deals with these problems is also addressed. In the next Section 4 we briefly demonstrate an application of RMM to relational modeling from the area of modeling temperature-dependent chemical properties.

The main focus of the paper is some initial results obtained recently from the work of Mrs. Fatena Awad, a PhD student under the supervision of this author. While a full report of these results will be co-published once the research is completed, the initial results seem to suggest some important conclusions with respect to the relative effectiveness of various families of distributions, commonly employed to fit distributions to data. These results and some discussion of their implications are the subject of Section 5.

We conclude with some summarizing comments in Section 6.

2. RMM- Introduction of the Basic Model and Variations

At the heart of RMM is a relational model, which describes a modeled response, Y , in terms of a linear combination of effects (denoted the Linear Predictor, η), which transmit systematic variation to the response, two possibly correlated normal errors, ε_1 and ε_2 , and a vector of parameters:

$$W = \log(Y) = (\alpha/\lambda)[(\eta+\varepsilon_1)^\lambda - 1] + \mu_2 + \varepsilon_2, \quad (1)$$

where $\{\alpha, \lambda, \mu_2\}$ are three parameters that need to be determined.

Assuming that the errors derive from a bi-variate normal distribution, and expressing ε_2 in terms of ε_1 plus an additive *independent* error, the RMM model becomes

$$W = \log(Y) = (\alpha/\lambda)[(\eta + \sigma_{\varepsilon_1} Z_1)^\lambda - 1] + \mu_2 + \sigma_{\varepsilon_2}[\rho Z_1 + (1-\rho^2)^{(1/2)} Z_2], \quad (2)$$

where σ_{ε_1} and σ_{ε_2} are the standard deviations of ε_1 and ε_2 , respectively, Z_1 and Z_2 are two *independent* standard normal variates, and ρ is the correlation between ε_1 and ε_2 .

Assuming arbitrarily $\eta=C$ (a constant), (2) becomes the quantile function of the RMM error distribution. Assuming further that $\rho=\pm 1$, we obtain from (2) the quantile function of Y , expressed in terms of the corresponding standard normal quantile.

Expressed in a re-parameterized form, (2) becomes (with $\eta=1$):

$$W = \log(Y) = \log(M) + [\alpha/(\lambda/S_1)][(1 + S_1 Z)^{\lambda/S_1} - 1] + S_2 Z], \quad (3)$$

where M is the median of Y (that is, $Y=M$ for $Z=0$), and $\{\alpha, \lambda, S_1, S_2\}$ are parameters that need to be determined. It may be shown that either S_1 or S_2 may be negative (but not both, find details in Shore, 2005, and references therein).

A variation of (3) with less parameters, which also provides good representation to variously-shaped distributions, is

$$W = \log(M) + (A/B)[\exp(BZ) - 1] + CZ, \quad (4)$$

where $\{A,B,C\}$ are parameters that need to be determined. For obvious reasons, the RMM quantile functions, (3) and (4), have been denoted, in some earlier references, Inverse Normalizing Transformations (INTs). Other versions of the RMM quantile function also exist (find details in the above reference).

For most applications, using (4) instead of (3) to model the quantile function of a r.v., Y , should be recommended. This is mainly for two reasons. First, when these quantile functions are fitted to data obtained from an unknown distribution, computer search for the parameters in (3) may occasionally result in imaginary values (that is, when $1 + S_1 Z < 0$). This may be troublesome. Secondly, assuming that M is estimated from the sample's median, (4) contains only three parameters while (3) contains four. This implies that in estimating the parameters of (4) via moment-matching, only the first three moments need to be estimated from sample data. The large sampling errors, associated with an estimate of the fourth moment (the kurtosis), is thus avoided. Maximum likelihood estimating procedures for (3) and (4) are detailed in Shore (2005).

Both (3) and (4) have been shown to deliver excellent representation for the quantile function of various distributions like the binomial, the Poisson, gamma, Weibull and the Extreme-Value distributions. Fitting to these distributions have been carried out by quantile matching, using non-linear least-squares. The accuracy obtained, as assessed by the preservation of the first four moments of the approximated distribution, has been shown to be satisfactory even for highly skewed distributions (skewness values ranging from zero to over eleven).

3. Motivation for the Development of RMM

The RMM model is derived from a set of axioms that seem to be of general enough character to allow RMM to provide general platforms for empirical modeling of both systematic variation and random variation. In fact, the development of RMM was essentially triggered by the author's strong conviction that current platforms for empirical modeling, like GLM (Generalized Linear Models), suffer from certain drawbacks that undermine their validity as general platforms for modeling. Some of these drawbacks and how RMM seems to respond to them are expounded in this section.

3.1 Transitions from modeling random variation to modeling systematic variation

All current platforms for modeling systematic variation have originated in models of random variation. Thus, linear regression has originated in the normal distribution, where it is assumed that the mean can be expressed as a linear combination of systematic effects, and likewise GLM has originated in the exponential family of distributions. Not surprisingly, the resulting relational models, especially those produced in the framework of GLM, carry little resemblance to relational models developed over many years in various disciplines of science and engineering. By contrast, RMM has been developed as a generalization of these models, with only one restriction: All models describe monotone convex (concave) relationship between the regressor (or the LP) and the response. This rather general characterization has served as a good departure point for the subsequent development of RMM. It seems that this origin of RMM is responsible for the cumulative experience we have thus far had with RMM which shows this approach to be so effective, producing models with goodness-of-fit fairly comparable to much more complicated empirical relational

models, nowadays commonly used in various application areas (like software reliability-growth modeling or chemical engineering; Refer for an example to the latter to Section 4).

RMM embodies the only general modeling approach, presently available, which has its roots in the area of modeling systematic variation rather than in the area of modeling random variation. Relative to corresponding models produced via GLM, models produced by RMM are therefore more compatible with those one may expect to find in various areas of science, engineering and operations management.

3.2 Transition from modeling systematic variation to modeling random variation

The quantile function of RMM, as developed in Section 2, is associated with the error structure of the RMM model. Since the latter has originally been developed for modeling systematic variation, one may say that that fitting RMM's quantile function to data represent a transition in the opposite direction to that experienced with linear regression and GLM, namely, the error distribution of a model, originally developed to model systematic variation, serves to model random variation. Since RMM contains many existent models as special cases, one may expect its quantile function, which essentially represents the errors associated with RMM, to deliver good representation to a wide spectrum of statistical distributions that one may encounter in practice. Initial results given in Section 6, where several families of distributions are compared in terms of the delivered goodness-of-fit, corroborate this conclusion, and demonstrate the efficacy of RMM among the families compared.

3.3 Changes in the error distribution due to systematic variation

It is a common experience, easily supported by arguments of a theoretical nature, that as systematic variation, transmitted to the response, causes it to vary over several orders of magnitude, the associated error distribution would tend to change in a profound fashion (namely, not only in terms of the parameters associated with the defined error distribution). In particular, as the response grows we expect a decoupling of the mean from the variance, which quite often leads to the asymptotic normality of the error distribution. This description requires that in constructing a relational model, the relationship between the mean and the variance should not be assumed to be constant. Estimating a GLM model, one is required a-priori to define such a relationship, which is assumed to remain constant over the complete range of

variation of the response. RMM does not have this drawback, as discussed in Shore (2005, Section 7.4).

3.4 Defining the model structure prior to model estimation

In all current approaches for modeling systematic variation (like linear regression, response transformation approaches and GLM) the model has to be specified in advance. Since for the RMM model two of the parameters determine the structure of the model (α and λ in eq. 1), the ultimate structure of the model is determined by the estimating procedure. As a result, more flexibility is expected in describing the data by the model, and as a result better goodness-of-fit. This property of RMM, namely, its ability to determine the final model as a result of the estimation procedure, is shared only by the Box-Cox transformation, where the non-linear structure of the final model (power or log transformation) may be determined by estimation. Likewise, in fitting RMM quantile function to data, the final shape of the quantile function is dictated by the data, and does not have to be specified in advance.

3.5 Four moment fitting

The practice of fitting distributions to data based on four-moment fitting is perhaps the most troubling aspect of the current state-of-the-art of modeling random variation. This is a most prevalent practice in distribution fitting. For example, most statistical packages, currently available, compute process capability indices for non-normal populations based on four-moment fitting of a member of the Pearson family (Clements' method, 1989) or the Johnson family. The large mean-squared-errors (MSEs) associated with estimates of high-degree moments has been repeatedly alluded to in the literature (for example, Karian and Dudewicz (2000, 2003), and Shore (2004a, 2005 and references therein). It has been emphasized that the use of estimates of high degree moments is risky and may be associated with unacceptably large sampling errors.

By contrast, RMM uses in a moment-matching procedure only moments of low degree (partial and complete). It has been shown that better estimates are obtained for small to medium sample sizes, thus evading the problem of the high MSE associated with four-moment matching (refer to Shore, 2005, Section 5.3.2, for details and additional relevant references).

4. An Example for Relational Modeling- Modeling Oxygen Vapor Pressure

This example is taken from the current PhD research of Benson-Karhi (2005), and displayed here with her permission. The performance of RMM for a wide range of vapor-pressure data was compared to that of the following existent models (for details about the first three models, relate to Daubert, 1998):

- **Antoine equation:**

$$\log(P) = A + \frac{B}{T + C} \quad (5)$$

where P is vapor pressure, T is temperature (in Kelvin) and {A, B, C} are parameters estimated by the regression of experimental data. This equation is widely used for vapor-pressure correlation (not only Oxygen).

- **Wagner's equation:**

$$\log(P_R) = \frac{a\tau + b\tau^{1.5} + c\tau^3 + d\tau^6 + e\tau^9}{T_R} \quad (6)$$

where {a, b, c, d, e} are adjustable parameters, T_R is the reduced temperature ($T_R = T/T_c$, where T_c is the critical temperature of the particular substance), P_R is the reduced pressure ($P_R = P/P_c$, where P_c is the critical pressure of the particular substance) and $\tau = (1 - T_P)$. This specific equation form was developed for Oxygen data only.

- **The extended Riedel equation:**

$$\log(P) = A - \frac{B}{T} + C \log(T) + DT^2 + \frac{E}{T^2} \quad (7)$$

where {A, B, C, D, E} are 5 adjustable parameters (not only for Oxygen data).

- **Selected model(s) by "Table Curve" (TC):**

This software (TC) selects the best model/models out of 4,000 different equations stored in its data-bank. Using "Model Selection" procedures surveyed in Burnham and Anderson (2004), where the AIC statistic is used for the final selection of the model, running TC with Oxygen data resulted in the following "best" model:

$$\log(P) = a + \frac{b}{T} + \frac{c}{T^2} + \frac{d}{T^3} + \frac{e}{T^4} + \frac{f}{T^5} + \frac{g}{T^6} \quad (8)$$

- **"Acceptable Model" recommended by DIPPR:**

DIPPR (Design Institute for Physical Property Data) is a widely used data-base for correlating physical and thermodynamic-responses (properties). It is today one of the

leading data-bases for physical properties and their modeling. It provides both data-sets and relational models to represent these data. Based on an examination of a large number of possible models, DIPPR offers for every combination of substance and property "The Acceptable Model", which is judged by the DIPPR scientific team to capture best the relationship between the response and the affecting factor (or factors). The "Acceptable Model" can be purely theoretical, purely empirical or a combination thereof. The latter case seems to be characteristic to most "Acceptable Models" that one can find in the DIPPR data-base.

The model currently recommended by DIPPR for vapor pressure is:

$$\log(P) = A + \frac{B}{T} + C \log(T) + DT^E \quad (9)$$

- **RMM**

A variation of (4) leads to the following version concerning vapor pressure data (note that a quantile function is used here for relational modeling; find further details in Shore, 2005, Ch. 17):

$$\log(P) = \log(\text{Median}P) + \frac{a}{b} \left[\exp\left(b \frac{T - \text{Median}T}{\text{Std}T}\right) - 1 \right] + a \frac{T - \text{Median}T}{\text{Std}T} \quad (10)$$

where MedianP and MedianT are the medians of the measured vapor pressure and temperature data, respectively, StdT is the standard deviation of the temperature data, and "a" and "b" are 2 adjustable parameters.

Characterization of data for all three gases analyzed in this research (Oxygen, Argon and nitrogen) are shown in Table 1 and the results of the comparison for Oxygen are shown in Table 2 (similar results were obtained for the other two gases). Lower AIC indicates a better fit. The three-parameter Antoine equation could not be fitted to data covering the wide temperature range of vapor pressure used in this example. It can be seen that the accuracy of the two-parameter RMM equation is significantly higher than that of the five-parameter DIPPR equation. Wagner equation provides the most accurate correlations for the vapor pressure of Oxygen, Argon and Nitrogen, but it should be noted that this equation was actually optimized (by stepwise regression) for the very same substances. From the results of this comparison, it can be concluded that the general purpose RMM competes favorably with the most accurate specific vapor-pressure equations for representing data covering a wide temperature range.

The same experience has been repeated more recently, when five substances and thirteen properties, provided by DIPPR, were analyzed via the RMM approach. Comparing the resulting goodness-of-fit relative to that obtained with the respective "Acceptable Models", as currently provided by DIPPR, has indicated, at least for this limited-scope preliminary study, that modeling via RMM most commonly provides better goodness-of-fit statistics than the existing models. Furthermore, no "guess-work" is required to find the structure of the best-fitting model since the RMM estimation procedure determines not only the parameters' values but also the very structure of the estimated model.

Table 1. Data Characterization- Vapor Pressure Data

	Oxygen	Argon	Nitrogen
Sample size (n)	177 ¹	57	68
Temp units	K	K	K
Temp range	90.188-154.581	83.804-150.651	63.148-126.2
Pressure units	MPa	bar	bar
Pressure range	0.10128-5.04337	0.6895-48.578	0.1252-34.002

Table 2. Comparison of Vapor-Pressure Correlation Equations for Oxygen Data

MODEL	No. of parameters	MSE	AICc
Antoine	3	-----	-----
Wagner	5	$6.08 \cdot 10^{-9}$	-3341
Riedel	5	$3.94 \cdot 10^{-8}$	-3011
TC	7	$1.04 \cdot 10^{-8}$	-3244
DIPPR	5	$2.98 \cdot 10^{-6}$	-2245
RMM	2	$1.49 \cdot 10^{-7}$	-2779

¹ The original data set contains 183 observations. Measurements 178-183 close to the critical point were found outliers with respect to most of the thousands of models been checked.

5. Comparing Five Families of Distributions for Goodness-of-Fit via the L_2 Norm

In this section we present some initial results obtained by Awad (2005), with her permission. In this part of the research, a set of five families of distributions were fitted to a representative sample of 20 distributions.

5.1 The set of families of distributions (used for fitting)

- Pearson Family, defined by the relationship:

$$\frac{df}{dx} = - \frac{(a - x)}{c_0 + c_1 x + c_2 x^2} f \quad (11)$$

- Burr Families of Distributions

Burr families are detailed in Table 2. Only Family XII is fitted in this analysis:

$$F(x) = 1 - (1 + x^c)^{-k}, \quad x > 0 \quad (12)$$

- GLD – The Generalized Lambda Family of Distributions (Karian and Dudewicz, 2000)

The quantile function, $Q(y)$ (in terms of the CDF, denoted regularly by y):

$$Q(y) = Q(y; \lambda_1, \lambda_2, \lambda_3, \lambda_4) = \lambda_1 + \frac{y^{\lambda_3} - (1-y)^{\lambda_4}}{\lambda_2}, \quad 0 \leq y \leq 1 \quad (13)$$

- Shore Family of Distributions (Shore, 1998)

The quantile function, x (in terms of the CDF, denoted regularly by P):

$$x = \begin{cases} A_1 \left(\frac{P}{1-P} \right)^{B_1}, & p < 1/2 \\ A_2 \left[\left(\frac{P}{1-P} \right)^{B_2} - 1 \right] + A_1, & p \geq 1/2 \end{cases} \quad (14)$$

Note that A_1 is the median ($P=1/2$). Therefore in fitting only three parameters need to be determined.

- RMM: As introduced by the quantile function in eq. 4.

Note that M is the median ($z=0$). Therefore in fitting only three parameters need to be determined. Also note that the Johnson family is a special case of RMM (Shore, 2004b).

Table 3. Burr Families of Distributions.

Family	Range	F(x) (The CDF)
I	$(0 < x < 1)$	x
II	$(-\infty < x < \infty)$	$(1 + e^{-x})^{-k}$
III	$(x > 0)$	$(1 + x^{-c})^{-k}$
IV	$(0 < x < c)$	$\left[1 + \left(\frac{c-x}{x}\right)^{1/c}\right]^{-k}$
V	$\left(\frac{-\pi}{2} < x < \frac{\pi}{2}\right)$	$(1 + ce^{-\tan x})^{-k}$
VI	$(-\infty < x < \infty)$	$(1 + ce^{-r \sinh x})^{-k}$
VII	$(-\infty < x < \infty)$	$2^{-k} (1 + \tanh x)^k$
VIII	$(-\infty < x < \infty)$	$\left(\frac{2}{\pi} \tan^{-1} e^x\right)^k$
IX	$(-\infty < x < \infty)$	$1 - \frac{2}{c[(1 + e^x)^k - 1] + 2}$
X	$(x > 0)$	$(1 + e^{-x^2})^k$
XI	$(0 < x < 1)$	$\left(x - \frac{1}{2\pi} \sin 2\pi x\right)^k$
XII	$(x > 0)$	$1 - (1 + x^c)^{-k}$

5.2 The approximated distributions (with their skewness and kurtosis values)

The list of 20 distributions approximated (fitted) by the five families of distributions, enumerated in Section 5.1, is given in Table 4.

Table 4. The set of 20 distributions fitted by the families of distributions detailed in Section 5.1.

Comment: Three of the distributions in this table are identical to those that appear in Karian and Dudewicz (2000) to allow easy comparison of distribution-fitting results.

#	Distribution	Skewness	Kurtosis
1	Chi-Square(5)	1.265	2.4
2	Log-Normal(0, 1/3)	1.0687	5.097
3	Exponential(0.5)	2	6
4	F-Ratio(5,10)	3.867	50.86153
5	Inverse-Gamma(3,5)	11.1287	471.557
6	Maxwell-Boltzman(4)	0.485693	0.108164
7	Inverse-Weibull(4,2)	5.53489	199.792
8	Meilke's Beta-Kappa(1,2,2)	18.6826	730.993
9	Pareto-II(3, 1)	14.6373	976936
10	Half-Normal(4)	0.995272	0.869177
11	Gomperts(2,3)	0.970789	0.631851
12	Standard Half-Logistic	1.54033	3.58374
13	Exponential-Power(2, 4)	-0.648501	0.110401
14	Chi(4)	0.405696	0.0592951
15	Pareto-III(1, 1)	2.53252	10.1756
16	Pareto(10, 5)	4.64758	67.8
17	Weibull(3,4)	0.168103	-0.270536
18	Rayleigh(0.5)	0.631111	0.245089
19	Noncentral-Chi-Square (4, 10)	0.817913	0.916667
20	Gamma(3, 2)	1.1547	2

5.3 The Analysis

The analysis included the fitting of the five families of distributions (Section 5.1) to the twenty distributions in the sample (Section 5.2). The objective was to find the best fit which minimizes the distributional distance between the approximated distribution and the fitted distribution, where as a measure for distance the L_2 Norm was used:

$$L_2 = \|f_{\theta}(x) - g(x)\|_2 = \left(\int (f_{\theta}(x) - g(x))^2 dx \right)^{1/2} \quad (15)$$

where $f_{\theta}(x)$ is the fitted density function, $g(x)$ is the density function of the true distribution and θ is a vector of parameters that minimizes (15). When the two distributions are identical, it can be shown that the L_2 Norm is identically zero.

Other measures of distances, like the “Kullback-Leibler divergence” measure (refer, for example, to Burnham & Anderson, 2000), were also used but subsequently discarded from further analysis.

To obtain the optimal parameters that minimize (15), MATHEMATICA[®] was used with the command NMinimize, activated to search for the optimal parameters. Values of L_2 at the optimal solution were used for subsequent statistical analysis in order to rank the various families of distributions in terms of their capability to represent well the sample of 20 distributions. Note that some of the distributions in Table 4 are special cases of the Pearson family. Therefore when all twenty distributions were analyzed, the Pearson family was excluded from the comparison. Conversely, for the Pearson family only 14 distributions were analyzed.

Altogether $4 \times 20 + 14 = 94$ distributional fittings were carried out.

5.4 Results

The experimental design called for analysis of variance with repeated measures. Therefore the paradigm for the analysis was Repeated Measure ANOVA With Fixed Effects, where the fixed effects are the families of distributions employed in the comparison. Various tests were conducted to ensure the validity of the assumptions underlying this analysis. Among the tests executed were a test for multivariate normality, Mauchly test for sphericity and other tests.

Table 5 presents averages and standard deviations for the L_2 norm for each of the five families of distributions fitted over the twenty approximated statistical distributions (16 for the Pearson family). Figure 1 displays the results graphically.

One may realize that RMM has both the smallest average ($1.148E-02$) and the smallest standard deviation ($1.1523E-02$).

Table 5. Summary statistics for the L_2 Norm, calculated for each family of distributions over the twenty distributions in the sample

		Statistics				
		L2 BURR	L2 GLD	L2 SHORE	L2 RMM	L2 PEARS
N	Valid	20	20	20	20	14
	Missing	0	0	0	0	6
Mean		.1378	3.192E-02	6.447E-02	1.148E-02	2.854E-02
Std. Deviation		.1130	3.817E-02	6.660E-02	1.523E-02	4.351E-02

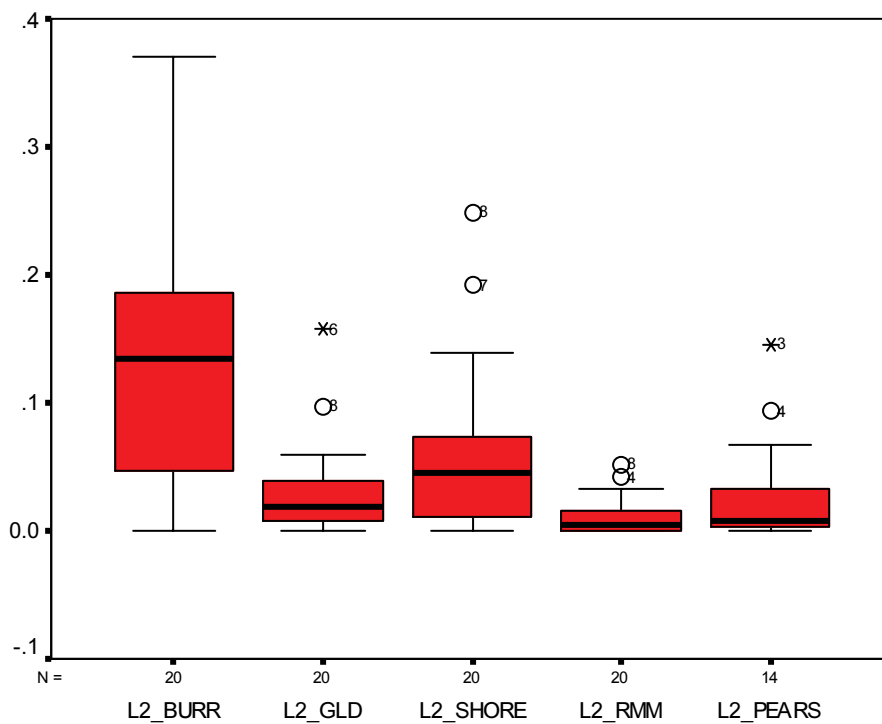


Figure 1. Box and Whisker diagram for the five families of distributions compared

6. Concluding Comments

This paper presents initial results from a large scale study in which the adequacy of various families of distributions, commonly used as general platforms for modeling random variation, has been evaluated. Some descriptive statistics are shown which indicate that it is possible to rank the various families. As shown by the results above, based on the L_2 Norm, and further validated by proper statistical analysis (not given here), RMM, Pearson and GLD, in that order, may serve as the best platforms for distribution fitting.

The results in this paper will be displayed in an extended fashion in an upcoming paper.

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