CMC-based Modeling – The Approach and Its Performance Evaluation

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(This article is affiliated to a blog entry, originally posted on ASA site)

1. INTRODUCTION

In earlier blog entries, the **Continuous Monotone Convexity (CMC)** property had been introduced as the "culprit" for the extreme effectiveness of the Box-Cox (BC) transformation (or, more precisely, for its inverse). I have emphasized that the inverse BC transformation (IBCT) delivers continuous presentation for the first *three* models ("steps") on the Ladder of Monotone Convex functions while the basic model of **Response Modeling Methodology (RMM)** delivers representation to the first *four* "steps". That model can be *generalized* to deliver representation to all models of the Ladder: adding two new parameters allows "climbing" three steps further on the Ladder. Furthermore, this iteration can be repeated at will to obtain ever more convex models. The number of models ("steps") belonging to the Ladder thus become potentially unbounded, restricted only by the number of parameters added to the basic RMM model. In other words, via a proper selection of parameters' values any conceivable degree of monotone convexity can be achieved.

In this article, affiliated to my January 2014 blog entry posted at the ASA site, I outline CMC-based modeling via RMM and review current literature that describes the performance of RMM modeling relative to models that have appeared in the literature of various scientific and engineering disciplines. More specifically, the objective of this article is twofold:

- To deliver a succinct introduction to the basic RMM model, as used for modeling random variation and for modeling systematic variation;
- To review published empirical evidence for RMM performance as a general modeling platform, capable of replacing published models either when parameters of the latter are known or when they are estimated from observational or Monte-Carlo-generated data.

Accordingly, the rest of this article is divided into two parts (apart from this Introduction):

In the first part (Section 2), the basic RMM model is introduced as a model of *systematic variation* (where the latter is expressed via a *linear predictor*, LP), and as a model of *random variation* (expressed as a general model for a normal-based quantile function). All terms used herewith are described in more detail later on, when the RMM model is expounded.

In the second part (Section 3), we review published empirical evidence for the capability of RMM models to replace current published models of *systematic variation*. We relate to models that have appeared in the relevant literature of various scientific or engineering disciplines. These models may be purely theoretical, purely empirical or semi-empirical. Empirical evidence for RMM performance, as published over the years, relates to two scenarios, associated with two different types of tests conducted to evaluate RMM performance:

- **Scenario I:** The parameters of the original model (to be substituted by a fitted RMM model) are known;
- **Scenario II:** The parameters of the replaced model are unknown (and need to be estimated, along with the RMM model, from either simulated data or from observational data).

Note that the two options lead to two different modes of assessing RMM performance (as a general modeling approach): In the first case (Scenario I), the functional distance between the original model and the fitted RMM model is minimized (via minimizing the L2 norm, a functional distance measure). In the second case (Scenario II), the quality-of-fit of the two models (the original and RMM) is compared using known measures for comparison of models, like mean-squared errors (MSE, if RMM is fitted as a mean model), mean-absolute-deviation (MAD, if RMM is fitted as a median model) and AIC.

In a future blog entry (and an affiliated article #4), we will review published empirical evidence for the capability of RMM models to replace current models of *random variation*, either when the latter represent distributions with known parameters or otherwise.

As is typical to all articles in this series, the technical detail is kept to minimum so that only the essential elements, required for understanding the approach and its evaluation, are addressed. Throughout the article, the reader is referred to relevant published papers for further details.

2. THE RMM MODEL

The basic RMM model is developed axiomatically in Shore (2005, Ch. 7). It is assumed that the response variable (the modeled variable, Y) experiences variation from two sources that interactively affect the response:

- Self-generated random variation (represented by a multiplicative normal random error, denoted ε_2), namely: $M(1+\varepsilon_2)$, where M is a constant (a parameter);
- Externally generated systematic and random variation, represented by an LP, η, and an additive normal random error, ε_1, respectively. This source of variation affects the response non-linearly.

It is assumed that ε_1 and ε_2 derive from a bi-variate normal distribution with correlation, ρ. Assuming further that $\varepsilon_2 << 1$, the original RMM model is:

$$\log(Y) = \mu + (\frac{\alpha}{\lambda})[(\eta + \varepsilon_1)^{\lambda} - 1] + \varepsilon_2 \ . \tag{1}$$

From this basic model, a re-parameterized RMM model is derived for the quantile of the distribution of Y, denote it by y, in terms of the LP (η) and the corresponding standard normal quantile, z (find details in Shore, 2005, 2011):

$$W = \log(\mathrm{y}) = \log(M_Y) + \left(\frac{a\eta^b}{b}\right)\left\{[1 + (c/\eta)\mathrm{z}]^b - 1\right\} + (d)\mathrm{z} + \varepsilon \ , \tag{2}$$

where M_Y is the response median (eq. 2 with z=0), ε is the model's random error and {*a,b,c,d*} are parameters. It is easy to show that the expression for the median, M_Y, is:

$$\log(M_Y) = \mu + \left(\frac{a}{b}\right)[\eta^b - 1] = \log(m) + \left(\frac{a}{b}\right)[\eta^b - 1], \tag{3}$$

where *m* is a parameter. Alternatively, assuming that in (1): $\varepsilon_1 << \eta$, we obtain, approximately:

$$W = \log(y) = \log(M_Y) + \left(\frac{a}{b}\right)\left[e^{b[\log(\eta) + \frac{cz}{\eta}]} - 1\right] + (d)\mathrm{z} + \varepsilon \ , \tag{4}$$

with M_Y as in (3). Re-parameterized for simplicity, (4) may be re-written:

$$W = \log(y) = \log(M_Y) + \left(\frac{a\eta^b}{b}\right)\left[e^{\frac{bz}{\eta}} - 1\right] + (d)\mathrm{z} + \varepsilon \ . \tag{4a}$$

Occasionally, a response location parameter, *L*, needs to be added, so that (2), (3) and (4a) become, respectively:

$$W = \log(\mathrm{y} - \mathrm{L}) = \log(M_Y - \mathrm{L}) + \left(\frac{a\eta^b}{b}\right)\left\{[1 + (c/\eta)\mathrm{z}]^b - 1\right\} + (d)\mathrm{z} + \varepsilon \tag{5}$$

$$\log(M_Y - L) = \mu + \left(\frac{a}{b}\right)[\eta^b - 1] = \log(m - L) + \left(\frac{a}{b}\right)[\eta^b - 1], \tag{6}$$

$$W = \log(y - L) = \log(M_Y - L) + \left(\frac{a\eta^b}{b}\right)\left[e^{\frac{bz}{\eta}} - 1\right] + (d)\mathrm{z} + \varepsilon \tag{7}$$

Various estimating procedures for (2)-(7) are detailed in Shore (2012).

If (3) is used to model the median (*z*=0), then apart from the parameters of the LP (η), this model requires estimating only two additional RMM parameters (since parameter *a* in (3) may be absorbed in the parameters η and μ). Also, the standard deviation of the (zero-mean) error, ε, needs to be estimated.

Assuming that η=Constant (namely, no systematic variation exists), we may set, without loss of generality: η=1, to obtain from (5) and (7) for the normal-based quantile function of the response, Y:

$$W = \log(\mathrm{y} - \mathrm{L}) = \log(M_Y - \mathrm{L}) + \left(\frac{a}{b}\right)\{[1 + c\,\mathrm{z}]^b - 1\} + (d)\mathrm{z} + \varepsilon \tag{8}$$

$$W = \log(\mathrm{y} - \mathrm{L}) = \log(M_Y - \mathrm{L}) + \left(\frac{a}{b}\right)[e^{bz} - 1] + (d)\mathrm{z} + \varepsilon \tag{9}$$

Note that the term "normal-based quantile" denotes herewith the percentile of the response, Y, in terms of the corresponding standard normal percentile.

Model (8) has served as an essential component for an RMM-based *general* model of random variation (Shore, 2013a). However, as will be detailed in a future article, (8) and (9) may practically replace normal-based quantile functions of known distributions with negligible loss in accuracy.

For a median model with a single covariate, *X*, eq. (6) may be forced to pass through a pre-selected point, (M_X, M_Y). This point may represent either the overall median point or any other central point that we wish the median model to pass through (namely, for this point: ε=0). The following simple median model is one option, obtainable from (6):

$$W = \log(Med - \mathrm{L}) = \log(M_Y - \mathrm{L}) + \left(\frac{a}{b}\right)\left[\left(\frac{x}{M_X}\right)^b - 1\right] + \varepsilon \quad , \tag{10}$$

where *Med* is the modeled median (as function of covariate, x).

If it is assumed that the distribution of the response, Y, is symmetrical (in which case the median is equal to the mean), this model may serve also as a mean model.

3. PUBLISHED EVIDENCE FOR RMM PERFORMANCE

Over the last decade, I have published, with colleagues or with research students, a large set of articles, aimed primarily to establish the RMM model as a general platform for modeling monotone convex relationships. This has been done in three forms:

[1] Approximating published models with an RMM model (via minimizing the L2 norm, a functional distance measure);

[2] Using data generated from a published mean model (assuming additive normal error), the RMM model and the data-generating model are estimated and compared;

[3] Using raw field data, the RMM model and the published model are concurrently estimated and compared.

In this section we deliver highlights of these comparisons, as published in various discipline-oriented journals over the last decade or so. We relate to five scientific and engineering disciplines:

* Chemical engineering (Section 3.1);

* Software quality engineering (specifically, software reliability-growth models; Section 3.2);

* Process capability analysis for skewed process distributions (Section 3.3);

* Ecology (Section 3.4);

* Ultra-sound-based fetal-growth modeling (modeling reference (population) fetal-growth curves, based on cross-sectional data; Section 3.5).

Published evidence for the performance of RMM as a general platform for modeling random variation will be reviewed in the next blog entry in this series.

3.1 Chemical Engineering

In a series of articles, published in various chemical-engineering oriented journals over the years 2002-2010, we (me with colleagues) have modeled fourteen temperature-dependent properties of pure substances (like oxygen or water), using models from three sources:

*A dedicated software, TableCurve2D (henceforth TC), which automatically fits mathematical functions to a given data set. At the time of analysis, TC had a database of nearly 3700 linear and non-linear functions, which it fits to a given data set, resulting in ranked models according to some goodness-of-fit criteria (note that linearity here refers to “linearity in parameters” and not necessarily to linearity in the regressor variables). A least-squares procedure is used to estimate the parameters. In our analyses of models derived with TC, a normal additive error with constant variance was assumed. This rendered the least-squares fitting, offered by TC at the time, into a maximum likelihood procedure. Proper steps were taken to ensure that this assumption was valid.

* A widely used data-base for correlating physical and thermodynamic-responses (properties), known as DIPPR (Design Institute for Physical Property Data; see details in *Rowley et al.*, 2006). It is today one of the leading data-bases for physical properties and their modeling, and it provides both data-sets and relational models to represent these data. Based on examining 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 (temperature). The "Acceptable Model" can be purely theoretical, purely empirical or a combination thereof. The latter case seems to be typical to most "Acceptable Models" that one can find in the DIPPR data-base. Note, that while TC provided, in this study, a particular model for each substance-property combination, DIPPR provided a uniform model for each property (though parameters' values differ between substances). RMM provided a uniform model (though with parameters-reduced variations) to all substances and all properties.

* RMM models, with three variations: a 2-parameter model, a 3-parameter model and a 4-parameter model. All RMM models were used as mean models (implying that fit is achieved by minimizing the sum of squared deviations, or MSE).

All three sources had provided models that were estimated and compared by two set of criteria:

- "Quality of Fit" criteria: these included MSE and AIC_c (corrected AIC);
- "Stability of Parameters" criteria: these included PRESS (PRediction Sum of Squares) and the relative length of the parameters' 95% confidence intervals (CI), namely: the value of the CI length divided by the estimate.

In Tables 1 and 2 below (which appear as Tables 16 and 17 in Benson-Karhi *et al.*, 2007), we summarize comparisons made with regard to modeling properties of Oxygen, Argon, Nitrogen and water. These tables also include summary results from a paper published three years later (Shore and Benson-Karhi*,* 2010).

Table 1. Frequency table of models' rankings (across all properties) relating to Goodness-of-fit Criteria (MSE and AIC_C).

	Goodness of fit (MSE, AIC_C)					
	Rank	"1"	"2"	"3"	Missing	Sum
Oxygen	TC	14	4	0	8	26
	DIPPR	0	6	12	8	26
	RMM	4	8	6	8	26
Argon	TC	10	2	0	14	26
	DIPPR	0	4	10	12	26
	RMM	4	8	2	12	26
Nitrogen	TC	15	3	0	8	26
	DIPPR	2	0	16	8	26
	RMM	1	15	2	8	26
Water	TC	18	3	3	2	26
	DIPPR	4	9	11	2	26
	RMM	10	8	6	2	26
SUM	TC	57	12	3	32	104
	DIPPR	6	19	49	30	104
	RMM	19	39	16	30	104

Table 2. Frequency table of models' rankings (across all properties) relating to Stability Criterion (PRESS)

	Stability (PRESS)					
	Rank	"1"	"2"	"3"	Missing	Sum
Oxygen	TC	5	2	0	6	13
	DIPPR	0	4	5	4	13
	RMM	4	3	2	4	13
Argon	TC	5	1	0	7	13
	DIPPR	1	2	4	6	13
	RMM	1	4	2	6	13
Nitrogen	TC	5	0	1	7	13
	DIPPR	2	2	5	4	13
	RMM	2	7	0	4	13
Water	TC	5	1	2	5	13
	DIPPR	5	4	3	1	13
	RMM	6	5	1	1	13
SUM	TC	20	4	3	25	52
	DIPPR	8	12	17	15	52
	RMM	13	19	5	15	52

Table 1 relates to "Quality of Fit" criteria and Table 2 to "Stability of Parameters" criteria (note that in the latter table, results relating to PRESS only are given). The tables display frequencies of ranking positions at which each model source has appeared in the various comparisons (using various criteria): rank "1" (the best), rank "2" and rank "3" (the worst).

We realize that, as expected, TC delivers best source of models since this source selects a different model for each substance-property combination (out of a huge data-base of available models). However, comparison between DIPPR and RMM shows RMM to deliver, on average, better models than those recommended by DIPPR (note the summary sections at the bottom of each table).

3.2 Software Reliability-growth Models

A major motivation for the use of models in software quality engineering is the ability of estimated models to predict the cumulative number of failures, N_t, given the history of testing-hours, t, invested in detecting software failures. The models are denoted *software reliability-growth models* since they assume that detecting an error (which results in failure) and removing it cannot result in the production of new error(s). To predict the cumulative number of detected errors as function of t, various models have been suggested. In Shore (2004, 2005, Ch. 16) I review these models, and then use a published data set, known as Musa's M_3 data set (Musa, 1979) to compare some of these models to an RMM model.

Figure 1 (appearing as Figure 16.4 in Shore, 2005 and as Figure 1 in Shore, 2004) shows scatter plots of residuals obtained from fitting three models:

Model 1: Suggested by Duane (1964), who had proposed the Power-Law to describe the process of detecting errors (refer also to Section 2.6 in Shore, 2005):

$N_t=\alpha t^{\beta}$, $\alpha,\beta >0$.

Model 2: Suggested by Xie and Zhao (1993):

$N_t = (\alpha)[\log(1+t)]^{\beta}$

Model 3: An RMM model.

Observing Figure 1 we realize that residuals from the estimated RMM model are more randomly (evenly) scattered around zero. Furthermore, the residuals standard deviations are 2988 for Model 1, 2962 for Model 2 and only 1471 (about half) for the RMM model.

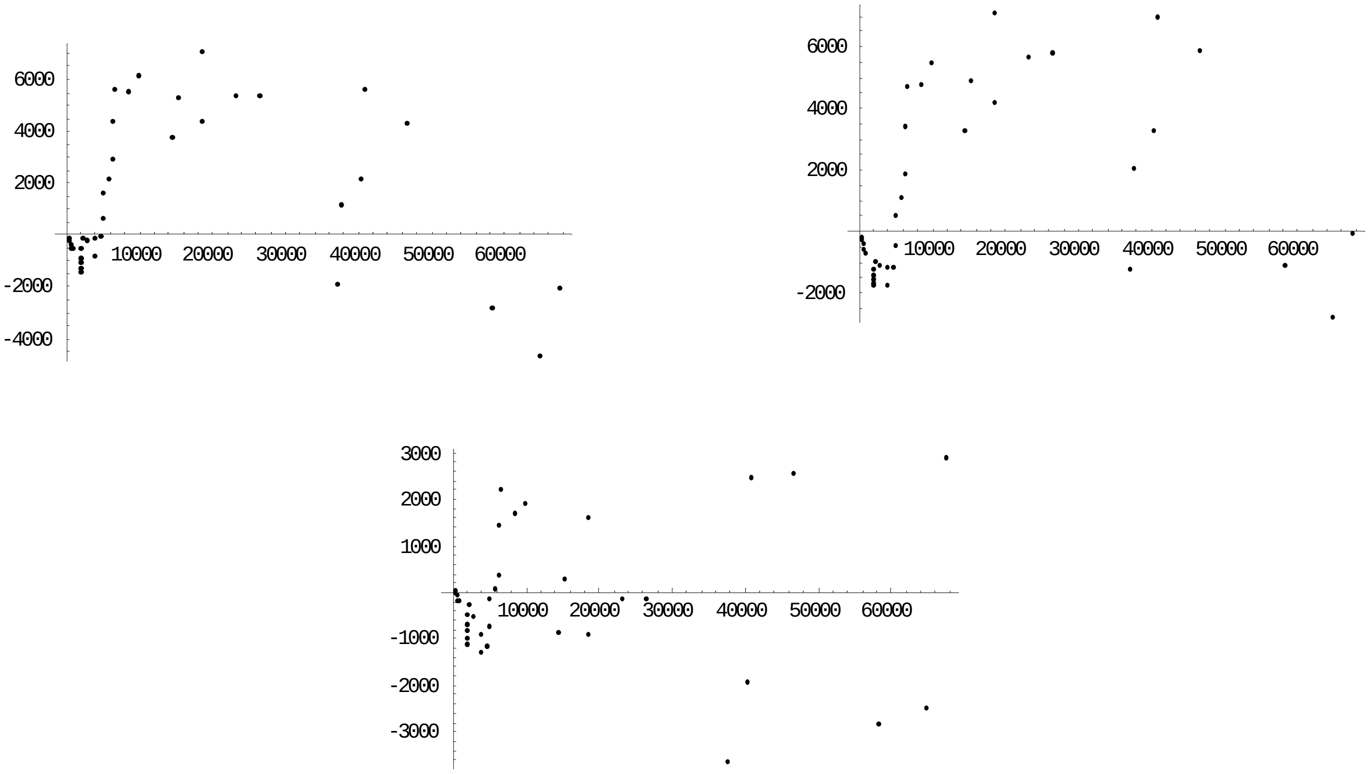

Figure 1. Scatter plots of residuals (vs. exact values of N_t) from fitting (clockwise) Model 1, Model 2 and Model 3 (RMM).

3.3 Process Capability Analysis (PCA) for Skewed Distributions

In a recent paper, based on research done in the framework of a PhD study, Shauly and Parmet (2011) compared the accuracy of Clements' approach (Celements,1989) to process capability analysis (PCA) for skewed distributions to the accuracy obtained from fitting an RMM model. Clements approach is based on fitting a Pearson distribution to the data and then use end-point percentiles of the fitted distribution as estimates for the end-points of the (unknown) process distribution. In the new study, Pearson was replaced by an RMM model, and the accuracy of estimates of C_p and C_{pU}, two process capability measures in wide use, is measured by the relative mean squared errors, MSE_R . For example, for an estimate of C_{pU}, $\hat{C}_{pU}$, we have for the relative MSE:

$$MSE_R(\hat{C}_{PU}) = \frac{MSE\left(\hat{C}_{PU}\right)}{\left(C_{PU}\right)^2} = E\left(\left(\frac{\hat{C}_{PU}}{C_{PU}} - 1\right)^2\right) = E\left(\left(\frac{\left(USL - \hat{X}_{0.5}\right)\left(X_{0.99865} - X_{0.5}\right)}{\left(USL - X_{0.5}\right)\left(\hat{X}_{0.99865} - \hat{X}_{0.5}\right)} - 1\right)^2\right),$$

where *USL* is upper specification limit, and X_p and $\hat{X}_p$ are the 100p-th percentile of the true process distribution and of the fitted (estimated) distribution, respectively.

Three factors that may affect the accuracy of RMM and Pearson as general platforms for PCA for skewed distributions are examined: the actual data-generating distribution (Weibull, lognormal, gamma), the skewness measure (0.5,1.25, 2) and sample size (50,300,2000). As quoted in the article's abstract, "The results show that RMM consistently outperforms Pearson, even for samples from gamma, which is a special case of Pearson. This implies that when observations are visibly skewed yet their underlying distribution is unknown, RMM estimators for C_p and C_{pU} take account of the information stored in the data more precisely than the Pearson model, and may therefore constitute a preferred distributional model to pursue in process capability analysis.".

Figure 2 is taken from Shauly's PhD work (which is also displayed in the published article). For the case of C_{pU}=2.0, it shows profile plots of $MSE_R(\hat{C}_{PU})$ by skewness and by fitting model (a separate plot for each combination of process distribution and sample size).

RMM models are the preferred choice (smaller MSE_R), relative to Pearson, in nearly any combination of distribution, skewness and sample size.

3.4 Ecology

Recently I have developed a new statistical process control (SPC) scheme for monitoring ecological processes (Shore, 2013b). The new scheme adopts the RMM model as a general platform for modeling the relationship between an SPC-monitored ecological response and covariates. To justify the use of RMM, I had to demonstrate that RMM may replace, with negligible loss in accuracy, ecological models that have appeared over the years in the professional ecological literature. This was done in two phases: In Phase I, current ecological models, with their parameters specified, have been approximated by the RMM model, using minimization of the L2 norm as a criterion both for the fitting process and for final evaluation of the *goodness-of approximation* obtained. Secondly (Phase II), data had been generated (simulated) from the current (published) ecological model and then both the data-generating model and the RMM model were estimated, and the *goodness-of-fit* of the two models compared (by various criteria used to compare models).

Plots of error curves for some of the ecological models approximated (in Phase I) by RMM appear in Figure 1 in Shore (2013b). Summary results, from the simulation study, conducted in Phase II in order to evaluate the performance of RMM relative to the data-generating models, appear in Table II therein. It is realized that although in most cases the RMM model has fewer

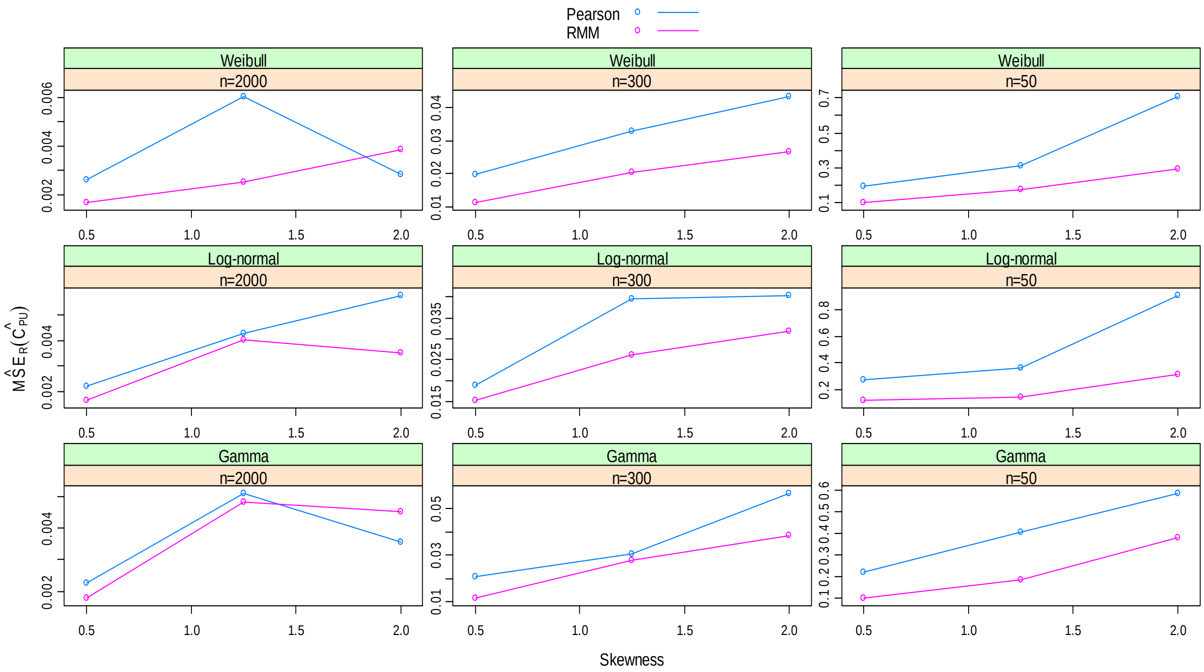

Figure 2. Profile plots of $\hat{MSE}_R\left(\hat{C}_{PU}\right)$ for $C_{PU} = 2.0$, by skewness and fitting model.

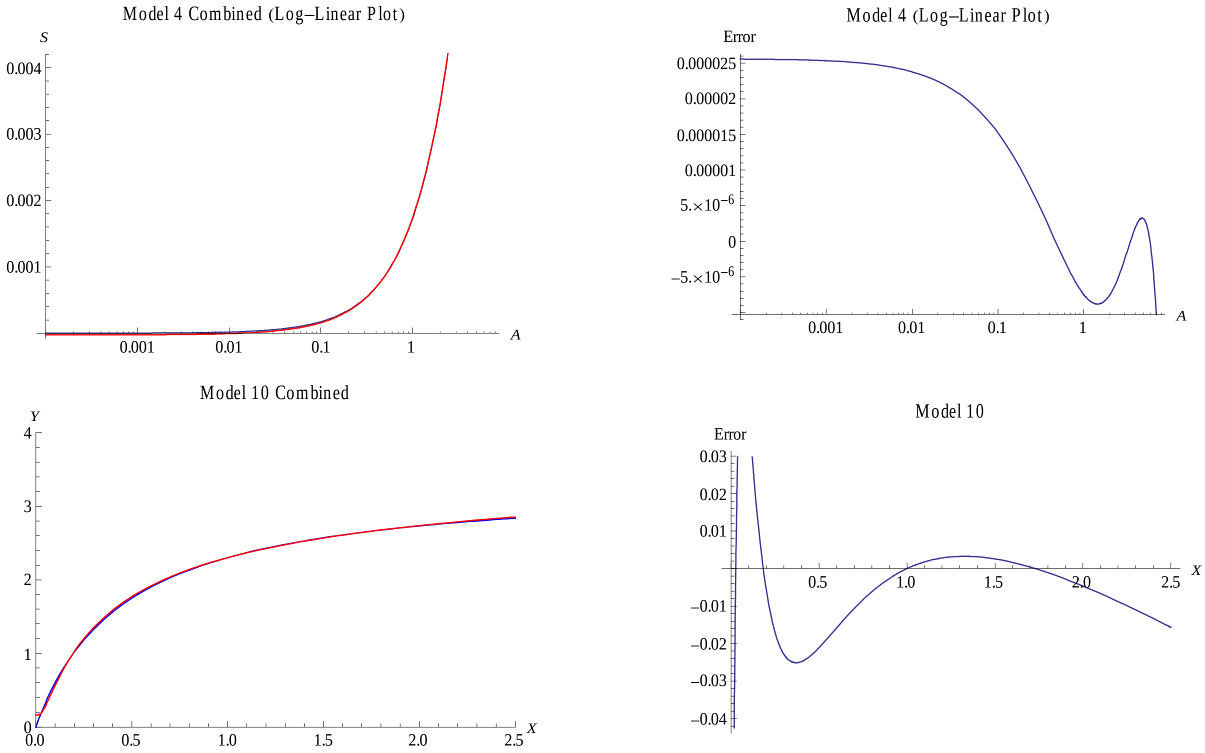

Figure 3. Two examples for ecological models that appear in Shore (2013b) (the combined original and fitted RMM models, on the left; error curves, on the right): Kobayashi Logarithmic model (Model 4, two upper plots) and the Hyperbolic Michaelis-Menten model (Model 10). Find more details therein.

parameters than the data-generating models, the fit of an estimated RMM model is either comparable or better.

Figure 3 displays two examples for the error curves obtained from approximating two ecological models by an RMM model.

3.5 Modeling fetal-growth reference curves

Fetal-growth reference curves serve as main tool to monitor fetal growth, based on ultra-sound (US) individual data. The latter refer to measurement data collected during pregnancy about the well-being of the growing fetus. These data relate to various measures collected during US examination, such as fetal head circumference (AC) or biparietal diameter (BPD). The reference curves display population (reference) centiles of these US measures as function of pregnancy age (gestational age, GA). They are constructed based on cross-sectional data collected from healthy pregnancies, and are assumed to represent the distribution (given GA) of the US measures in the population of healthy pregnancies.

Various models have been suggested to represent these percentile curves. The majority of the models are based on polynomials modeling the mean with the added assumption of normality (possibly with varying GA-dependent standard deviation).

In a recent study, the results of which are reported in as-yet unpublished article (Benson-Karhi *et al.*, 2013), we have examined the adequacy of RMM as a general platform to model fetal-growth reference curves. To conduct this examination, we have collected models that have appeared in the literature for the mean and fitted an RMM model to each, in an attempt to examine how well the RMM model can approximate these models. Additionally, two most commonly used models were tried as alternative general modeling platforms. The three models are:

Model 1: An RMM model (a variation of eq. (9)):

$$\log(y-L)=\log(M_y-L)+[\frac{a}{b}(e^{bz}-1)+cz],$$

where y is the biometric parameter at GA=x, z equals $(x-M_x)/M_x$ so that the model passes through point (M_x,M_y), $\{a,b,c\}$ are parameters and L is a response location parameter.

Model 2: Hadlock *et al.* (1984) polynomial models (henceforth denoted Hadlock models):

For HC and BPD: $y=a+bx+cx^3$

For AC and FL: $y=a+bx+cx^2$,

where x is the value of GA and *{a,b,c}* are parameters.

Model 3: Snijders & Nicolaides (1994) logarithmic polynomial models (henceforth the SN models):

$$\text{For HC, BPD and AC: } \log_{10}(y+k) = a + bx + cx^2$$
$$\text{For FL: } y^{0.5} = a + bx + cx^2 \quad ,$$

where {*k,a,b,c*} are parameters.

A set of 47 population mean equations that have appeared in the literature were approximated by the three models (RMM, Hadlock models and SN models). The approximating procedure minimized the L2 norm. Since the latter is not scale invariant, and in order to be able to compare goodness-of-approximation of RMM to other approximating models over all 47 approximated models and all US measures, we have defined a new scale-invariant measure, the *R* index:

$$R = \log\left[\frac{L2^{*}(\text{RMM})}{L2^{*}(\text{non-RMM})}\right] ,$$

where L2* is the minimized L2 and R is the log of the ratio of the L2* values obtained for a given combination of an RMM and a non-RMM (Hadlock or SN) *approximating* models, for a specified *approximated* model.

Note that if the RMM model achieves better goodness-of-approximation (smaller L2*), relative to a non-RMM model, one expects: R<0.

Figure 4 displays values of *R*, representing 69 comparisons, which have been conducted, of RMM with each of the other two competing models (Hadlock or SN): 30 comparisons with Hadlock model and 39 comparisons with SN model. We realize that all R values are negative, implying that for each approximated model, the fitted RMM resulted in better representation of the approximated model than that obtained by fitting either Hadlock or SN models.

Plots of error curves for all combinations (of RMM and non-RMM approximating models), and for all models approximated, are given in the Supplementary Material of the afore-cited article. Two examples are given in Figure 5.

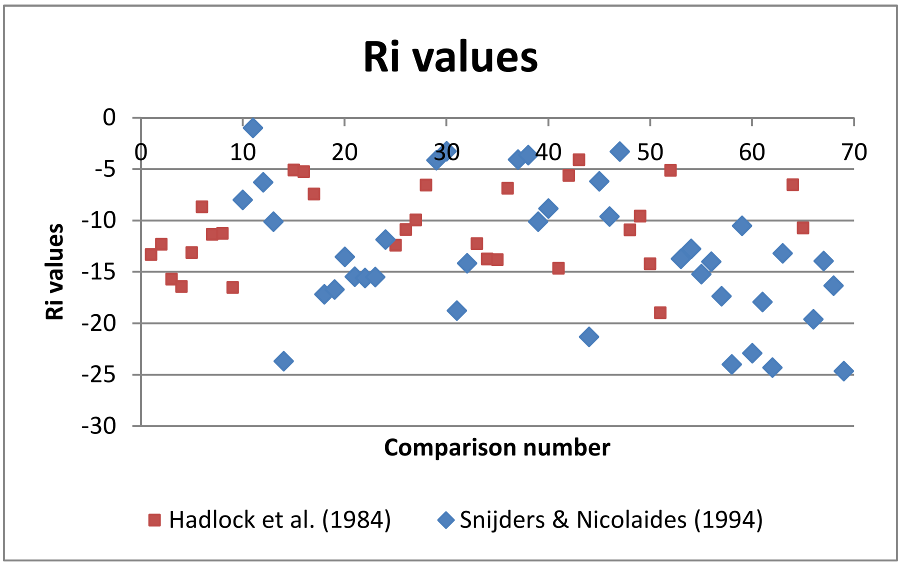

Figure 4. Values of *R* representing the 69 comparisons of RMM with each of the other two competing models: Hadlock model and SN model. Comparisons relate to several US fetal-growth measures.

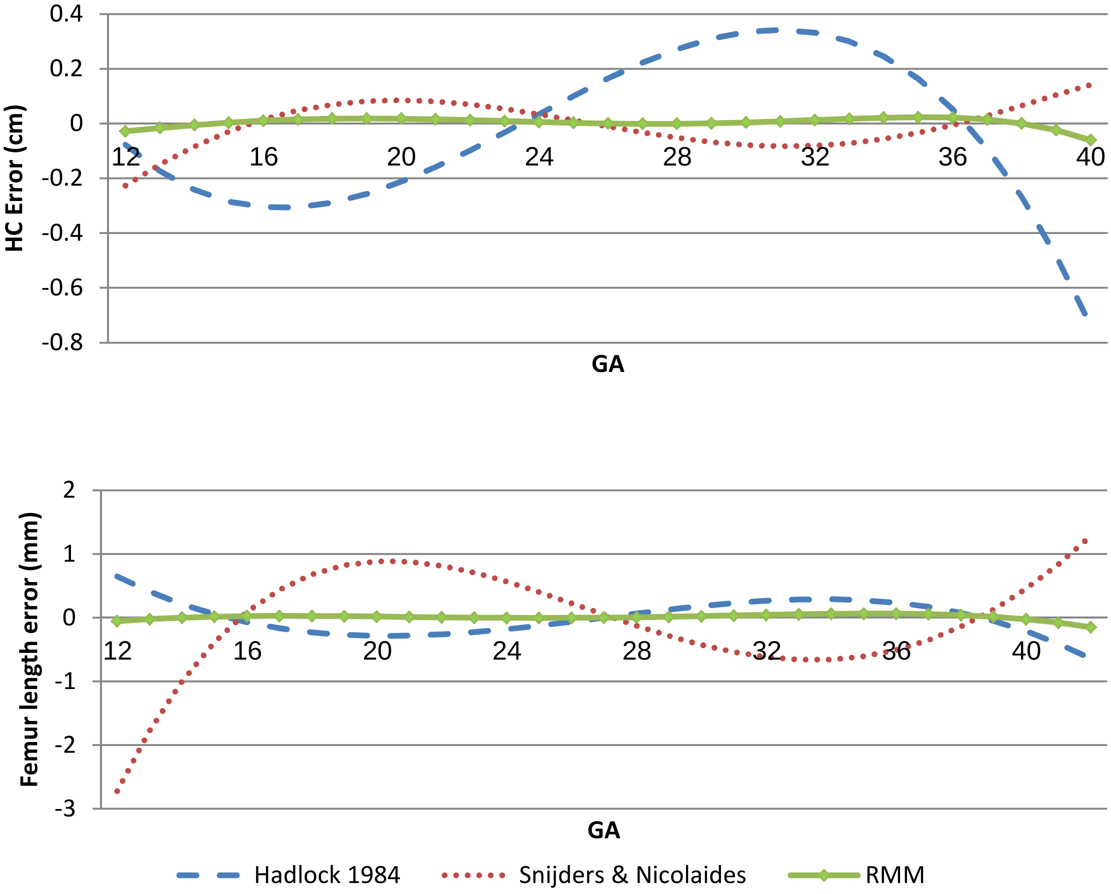

Figure 5. Two examples for the error curves obtained from approximating existent fetal-growth curves by Hadlock, SN and RMM models: Leung *et al.* (2008) model for HC (upper plot) and Chitty *et al.* (1994) model for FL. (GA is gestational age; *mm* and *cm* is millimetre and centimetre, respectively)

4. CONCLUSION

In this article I have reviewed published articles (and one under review), in which I have compared, sometimes with colleagues, the performance of RMM as a general platform for modelling monotone convex relationships, relative to models that have appeared in the relevant literature. These comparisons indicate that RMM, most likely due its unique CMC property, may serve well as a general modelling platform in scenarios where model mis-specification may potentially result in harmful consequences or when a general (universal) model is highly desirable.

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