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Working Paper CEMOTEV n° 05-2017

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Abstract The Cornish–Fisher expansion is a simple way to determine quantiles of non-normal distributions. It is frequently used by practitioners and by academics in risk management, portfolio allocation, and asset liability management. It allows us to consider non-normality and, thus, moments higher than the second moment, using a formula in which terms in higher-order moments appear explicitly. This paper has two primary objectives. First, we resolve the classic confusion between the skewness and kurtosis coefficients of the formula and the actual skewness and kurtosis of the distribution when using the Cornish–Fisher expansion. Second, we use the response surface approach to estimate a function for these two values. This helps to overcome the difficulties associated with using the Cornish–Fisher expansion correctly to compute value at risk (VaR). In particular, it allows a direct computation of the quantiles. Our methodology has many practical applications in risk management and asset allocation.

Keywords: Cornish–Fisher Expansion, Response Surface Methodology, Quantiles, Value at Risk, Expected Shortfall

JEL codes: C15, C44, C46, D81, G32.

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1 Introduction

Here, we propose an advanced approach to calculating approximate quantiles using the Cornish–Fisher (CF) expansion. We focus on the difference between the moments of the original distribution and those of the transformed distribution in order to resolve the difficulties of using the CF expansion. This study is in line with the work of MacKinnon (2010), Maillard (2012), and Amédée-Manesme et al. (2015). The approach and numerical distribution function obtained in this study can be used to compute quantiles, Value at Risk (VaR), the Expected Shortfall (or conditional value at risk; $CVaR$), and other critical values. The general principle of our work is to replace the original system of equations with an approximated (simpler) function, estimated using the response surface methodology, that is not as time consuming to use.

CF expansion is part of the Johnson distributions’ family class (see Johnson, 1949). The Johnson system covers different families of distribution and can in particular take account of the four first moments of a distribution. The Johnson’s transformation has the flexibility to match any feasible set of values for the mean, variance, skewness, and kurtosis. This class of transformation can be extended by considering all possible regular transformations of the standard Gaussian distribution among which CF or Gramm–Charlier as illustrated by Yeo & Johnson (2000); Naguez & Prigent (2017). This family of probability distributions can be independently calibrated to the four first moments of data. The advantage of the Johnson distributions is that quantiles of these distributions only depends on the quantiles of a standard normal random variable. In this line, the CF expansion is an approximation of the quantiles of a distribution using polynomials in the quantiles of a gaussian distribution with coefficients depending on the moments of the distribution under scrutiny.

Maillard (2012) highlights the difficulties of using the CF expansion correctly. In particular, he explains that two pitfalls should be avoided when using the CF expansion: the domain of validity of the formula (see also Amédée-Manesme et al., 2015), and confusion over the skewness and kurtosis parameters of the formula and those of the original distribution.¹ However, the solution proposed by Maillard (op. cit.) is restrictive in practice because it requires solving a numerically complicated equation, which is time consuming. Following the approach of MacKinnon (2010) for computing the critical values of cointegration tests, we rely on the response surface methodology (RSM). The general principle of the RSM is to replace the original estimation/computation with a different, but suitable function that is a polynomial.² The reliability level is then calculated using the classic techniques. This allows the direct computation of the CF values. Once the function(s) are estimated, this approach does not require a specialized computer program, is easily implementable, and is less time consuming than automated algorithm solvers. Our approach should be relevant for many practical purposes, but particularly for VaR or $CVaR$ computations.

Informally, Value-at-Risk is the largest percentage loss, for a given probability (confidence level), likely to be suffered by a portfolio position over a given holding period. In other words, for a given portfolio and time horizon, and having selected the confidence level $\alpha \in (0, 1)$, VaR is defined as a threshold value, assuming no further trade, such that the probability that the mark-to-market loss in the portfolio exceeds this VaR level is exactly the preset probability of the loss α . Note that VaR does not give any information about the likely severity of the loss by which its level will be exceeded. Thus, it is a quantile of the projected distribution of losses over the target horizon, in that if α is taken to be the confidence level, then VaR corresponds to the α quantile. By convention, this worst loss is always expressed as a positive percentage in the manner indicated. Thus, in formal

¹ In addition, Aboura & Maillard (2016) use the Cornish–Fisher expansion to revisit the pricing of options, in a context of financial stress, when the underlying asset’s returns display skewness and excess kurtosis. They derive an exact formula allowing for heavy tails.

² Other possibilities exist, but are not covered in this context.

terms, if we take L to be the loss ($L = E(V) - V_\alpha$), measured as a positive number, and α to be the confidence level, then VaR can be defined as the smallest loss (in absolute value), such that:

$$P(L > VaR) \leq \alpha. \quad (1)$$

A more detailed definition of VaR can be found in Jorion (2007).³

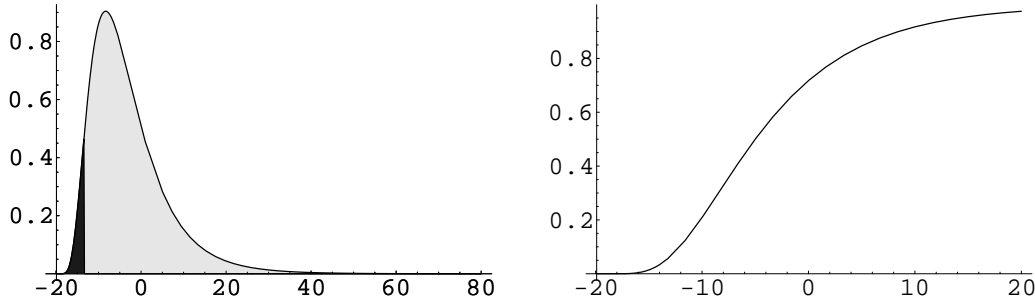


Fig. 1: Illustration of VaR for pdf and cdf

Figure (1) illustrates how to determine the VaR for a probability distribution with a density (pdf). For a given threshold α , VaR_α is the opposite of the quantile q_α of the distribution: the highest (“best”) value such that the probability of being below this value is smaller than α .

Figure (2) shows the pdf of returns and the pdf of returns conditional on exceeding the VaR. Two statistical models are considered for modeling the position: the Gaussian distribution, which has thin tails, and the Pareto–Levy distribution, with “fat” tails that decrease by a power. The two distributions have parameters such that they have the same VaR.

As shown, VaR is a risk measure that considers only the probability of a loss, not the size of a loss. Moreover, VaR is usually based on an assumption of normal asset returns, and has to be carefully evaluated when there are extreme price fluctuations. Furthermore, VaR may not be convex for some probability distributions. Owing to these deficiencies, other risk measures have been proposed, including the *expected shortfall (ES)*, as defined in Acerbi & Tasche (2002b), also called *conditional value at risk (CVaR)* in Rockafellar & Uryasev (2002) and *TailVaR* in Artzner et al. (1999). Note that in Acerbi & Tasche (2002a), several risk measures related to ES are considered and the coherence of ES is proved.

The ES can be expressed as follows (see Acerbi & Tasche, 2002b): Let \overleftarrow{F}_X be the generalized inverse of the cdf F_X of X defined by:

$$\overleftarrow{F}_X(p) = \sup \{x \mid F_X(x) < p\}.$$

³ In terms of gains rather than losses, the VaR at confidence level α for a market rate of return X , with a distribution function $F_X(x) \equiv P[X \leq x]$ and quantile at level α denoted as $q_\alpha(X)$, is

$$-VaR_\alpha(X) = \sup \{x : F_X(x) \leq \alpha\} \equiv q_\alpha(X).$$

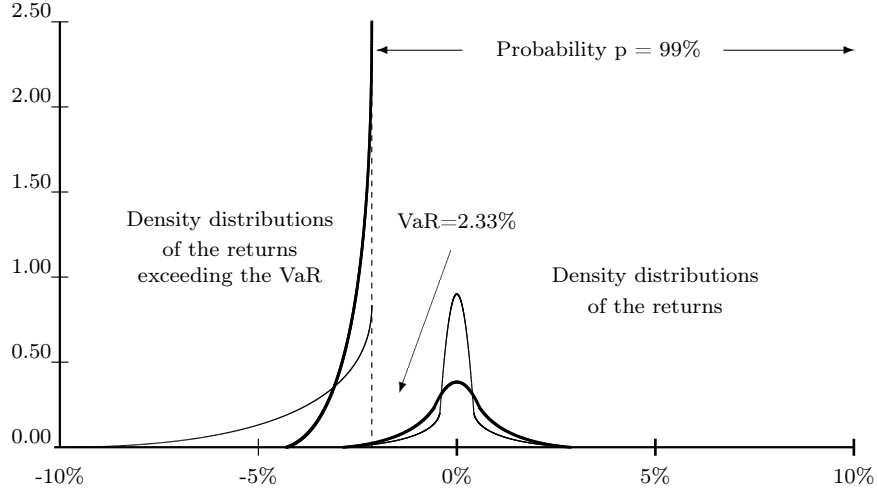


Fig. 2: Level of returns for Gaussian and stable Paretian distributions with the same VaR

Then, the ES is defined as the average in probability of all possible outcomes of X in the probability range $0 \leq p \leq \alpha$:

$$ES_{\alpha}(X) = -\frac{1}{\alpha} \int_0^{\alpha} \overleftarrow{F}_X(p) dp. \quad (2)$$

Then, for continuous cdf, the ES is given by:

$$ES_{\alpha}(X) = -(\mathbb{E}[X | X \leq q_{\alpha}(X)]), \quad (3)$$

where $q_{\alpha}(X)$ is the quantile of X at the level α .

Figure (2) illustrates how two probability distributions can have the same VaR, even though one is thin-tailed (the Gaussian case) and the other is fat-tailed (the Pareto–Lévy case). In this example, the VaR corresponding to a 99% probability of overshoot is equal to 2.33% of the value of the position. Nevertheless, a comparison of the expected shortfalls shows different risk levels.

Evaluating the marginal impacts of positions on risk measures and regulatory capital is a key part of risk management analyses (see, for example, Jorion, 2007).

Over the past few years, the popularity of downside risk measures (including VaR) has been increasing. Today, these metrics are replacing the standard deviation when evaluating the risks of investments. The reason behind the growing interest in downside risk measures is the choice of many regulators (Basel and Solvency) to rely almost solely on metrics such as VaR , or its derivative, $CVaR$, when determining required capital. Indeed, the crucial step in the worldwide adoption of VaR was the Basel II Accord of 1999, which resulted in a nearly complete adoption of the measure (Basel III must be applied by 2019). More recently, Solvency II regulations (for insurers in Europe) proposed using VaR as a reference measure in determining required capital. The Basel Accord requires that banks recalculate their VaR periodically and always maintain sufficient capital to cover the losses projected by VaR . Unfortunately, there is more than one measure of VaR , because volatility, a fundamental component of VaR , remains latent. Therefore, banks must use several VaR models, at least for backtesting purposes, and so must compute a range of prospective losses.

In this paper, we do not directly address the appropriateness of *VaR* as a risk estimator, nor the adequacy of this measure for risk budgeting purposes. It suffices that regulators have seen fit to choose a *VaR* measure for required economic capital calculations, and that its computation is mandatory for all regulated practitioners. The same holds for *CVaR*. Thus, *VaR* and *CVaR* are essential research subjects and of considerable interest to a broad spectrum of academics.

Cornish & Fisher (1938) established the expansion that bears their names. In the case of smooth random variables, it is possible to obtain an explicit expansion for any standardized quantile of the true distribution as a function of the corresponding quantile of the unit normal approximation introduced above. This Cornish–Fisher expansion is then a simple polynomial function of the corresponding unit normal quantile, where the coefficients of each resulting term are functions of the moments of the true distribution under consideration.⁴ For instance, denoting the Gaussian and the resulting Cornish–Fisher quantiles as z_α and $z_{CF,\alpha}$, respectively, we obtain the following expression for the normalized Cornish–Fisher quantile:⁵

$$z_{CF,\alpha} = z_\alpha + \frac{1}{6}(z_\alpha^2 - 1)S + \frac{1}{24}(z_\alpha^3 - 3z_\alpha)(K - 3) - \frac{1}{36}(2z_\alpha^3 - 5z_\alpha)S^2, \forall \alpha \in (0, 1), \quad (4)$$

where S and K denote the skewness and kurtosis coefficients, respectively, of the true distribution.⁶ The corresponding modified Cornish–Fisher quantile is then simply:

$$q_{CF,\alpha} = \mu + z_{CF,\alpha} \sigma_{CF}, \quad \forall \alpha \in (0, 1),^7, \quad (5)$$

and the expression for *VaR* is:

$$VaR_{CF,\alpha} = -q_{CF,\alpha} \quad \forall \alpha \text{ such that } q_{CF,\alpha} < 0. \quad (6)$$

Thus, the Cornish–Fisher expansion aims to approximate the quantile of a true distribution by using higher moments (skewness and kurtosis) of that distribution to adjust for its non-normality. Since the moments of the true distribution can be estimated in standard fashion by the sample skewness S and the sample kurtosis K , these values can then be substituted into equation (4) to estimate the unknown quantiles (*VaR*) of the true distribution. As demonstrated in Amédée-Manesme et al. (2015), the Cornish–Fisher approach leads to approximations closer to the true law than does the traditional Gaussian approach.

Therefore, the Cornish–Fisher expansion allows us to consider higher-order characteristics of the distribution when calculating quantiles, so that risky assets exhibiting non-normal distributions can be treated accurately. Thus, the Cornish–Fisher approach offers several advantages. First, it is comparatively easy to implement. Second, it allows for skewness and kurtosis in the *VaR* estimation, unlike the usual Gaussian approximation. Third, the approach makes no assumption about the time scale and so can be repeated over time.⁸ This renders the approach particularly relevant for, say, regulatory purposes. Indeed, the technique is independent of the nature of the underlying distribution and, thus, of its evolution. Therefore, it can be used regardless of the changes in this

⁴ This approximation is based on the Taylor series developed, for example, by Stuart & Ord (2009).

⁵ At the third order, the approximation is: $\forall \alpha \in (0, 1), z_{CF,\alpha} = z_\alpha + \frac{1}{6}(z_\alpha^2 - 1)S$.

⁶ It is straightforward to show that in the presence of an underlying Gaussian distribution ($S = 0$ and $K = 3$), equation (4) reduces to the Gaussian quantile. Thus, the Cornish–Fisher expansion can obviously be used when the distribution is normal).

⁷ Following Maillard (2012), $\sigma_{CF} = \frac{\sigma}{\sqrt{1 + \frac{1}{96}K^2 + \frac{25}{1296}S^4 - \frac{1}{36}KS^2}}$

⁸ However, exact distributions have advantages as well: they enable Monte Carlo simulations and, thus, allow for the direct computation of *VaR*.

distribution as the result of new, non-systematic events. This point is fundamental for risk management, where, as in accounting, one of the basic criteria is the “consistency principle,” requiring that a company must use the same risk measurements methods from period to period. Fourth, estimations using the Cornish–Fisher expansion do not require a large amount of data. For a *VaR* computation, the relevant quantiles need to be estimated. With a sufficiently large data set, we can use a straightforward empirical quantile. However, when available data are modest, resorting to Cornish–Fisher may be useful.⁹ If the return series is skewed and/or has abnormal tails (kurtosis), Cornish–Fisher estimates of *VaR* are more appropriate than traditional methods because, despite having to determine skewness and kurtosis, the method only requires modest amounts of data.

The Cornish–Fisher expansion owes its popularity in practice to its precision and explicit form, which make it straightforward to compute and interpret. Although it has proven to be a useful technique, because it is usually truncated at the third order (see appendix B), its use presents two major pitfalls: (i) the resulting approximations of the distribution and quantile functions can be non-monotone if the parameters do not meet the domain of validity; and (ii) the skewness and the kurtosis of the Cornish–Fisher expansion are generally not those of the true distribution, which can lead to confusion. Resolving these two issues requires that we combine the works of Chernozhukov et al. (2010) and Maillard (2012). We do so using a so-called rearrangement procedure (i) with a correction of the parameters (ii). This leads to the correct use of the Cornish–Fisher expansion.

(i) In fact, the resulting approximations of the distribution and quantile functions can be non-monotone. There are constraints on the permitted values of the true distributions’ moments so that the Cornish–Fisher expansion itself yields a well-defined distribution (for more details, see equation 24 in appendix B). This is due to the third-order truncation of the Cornish–Fisher expansion and the fact that the polynomials involved in the expansion need to be monotone. The non-monotonic behavior can lead to incorrect results (as illustrated by Amédée-Manesme et al., 2015, in Figure 2). Indeed, in such a case, the quantile at a higher threshold can be smaller in absolute terms than the one at a smaller threshold ($|q_{\alpha_1}| < |q_{\alpha_2}| \mid \forall \alpha_1 > \alpha_2$), which is obviously unpalatable for any cumulative distribution function, and even less desirable when it is used for risk measurement. A solution to this issue has been proposed by Chernozhukov et al. (2010), who suggested using a rearrangement procedure restoring the monotonicity of the approximation. The rearrangement procedure is a sorting operation: the previously obtained values are simply sorted in increasing order. Furthermore, according to Chernozhukov et al. (2009), in addition to restoring monotonicity, the rearrangement improves the estimation properties of the approximation. The resulting improvement is due to the fact that the rearrangement necessarily brings the non-monotone approximations closer to the true monotone target function. This point has already received attention in the literature (Amédée-Manesme et al., 2015).

(ii) Another difficulty associated with the use of the Cornish–Fisher expansion, truncated at the third order, is confusion between the skewness and kurtosis parameters of the formula (denoted here as S_c and K_c , respectively) and those of the underlying true distribution (S and K , respectively). This can lead to considerable mis-estimation of quantiles. Though this point has already been raised by Maillard (2012), it does not seem to have received sufficient attention elsewhere in the literature. The author presents a solution to the problem by computing the correct moments of the distribution resulting from the Cornish–Fisher expansion. This leads to the following true skewness (S , equation 7) and true kurtosis (K , equation 8) parameters (the technical details are available in the study by Maillard, 2012)¹⁰:

⁹ The 0.5% *VaR* of the Solvency II regulation requires a minimum of 17 years of data (17 years = 204 months).

¹⁰ Maillard (2012) computes the moments of the fourth-order Cornish–Fisher inverse expansion. The equations presented here correct a misprint and write S and K as functions of S_c and K_c

$$S = \frac{S_c - \frac{76}{216}S_c^3 + \frac{85}{1296}S_c^5 + \frac{1}{4}K_c S_c - \frac{13}{144}K_c S_c^3 + \frac{1}{32}K_c^2 S_c}{\left(1 + \frac{1}{96}K_c^2 + \frac{25}{1296}S_c^4 - \frac{1}{36}K_c S_c^2\right)^{1.5}}. \quad (7)$$

$$K = \frac{\left[\begin{aligned} &3 + K_c + \frac{7}{16}K_c^2 + \frac{2}{32}K_c^3 + \frac{31}{3072}K_c^4 - \frac{7}{216}S_c^4 - \frac{25}{486}S_c^6 + \frac{21665}{559872}S_c^8 \\ &- \frac{7}{12}K_c S_c^2 + \frac{113}{432}K_c S_c^4 - \frac{5155}{46656}K_c S_c^6 - \frac{7}{24}K_c^2 S_c^2 + \frac{2455}{20736}K_c^2 S_c^4 - \frac{65}{1152}K_c^3 S_c^2 \end{aligned} \right]}{\left(1 + \frac{1}{96}K_c^2 + \frac{25}{1296}S_c^4 - \frac{1}{36}K_c S_c^2\right)^{1.5}} - 3. \quad (8)$$

As demonstrated by Maillard (2012), proper use of the Cornish–Fisher expansion requires that we invert these relations. This way, the correct skewness and kurtosis can be entered into the expansion (the correction is required because the Cornish–Fisher expansion is an approximation of order 3). This can be done numerically.

Note that S and K are the true values of skewness and kurtosis we are working with, while S_c and K_c are the values we will use in the CF transformation in order to obtain the correct moments after the transformation. Maillard denotes the functions f and g , such that:

$$K = f(K_c, S_c) \quad (9)$$

and

$$S = g(K_c, S_c). \quad (10)$$

In practice, the reverse relationships are needed, where S_c and K_c belong in the incoming set of the searched functions. Following Maillard (2012), we denote these functions as φ and ψ , respectively:

$$K_c = \varphi(S, K) \quad (11)$$

and

$$S_c = \psi(S, K). \quad (12)$$

Here, we propose using the response surface methodology (RSM) to compute the Cornish–Fisher value at risk (hereafter, *CFVaR*). This allows us to estimate a function to directly estimate S_c and K_c and, thus, to overcome the difficulty resulting from the non-explicit form of the functions φ and ψ . However, the nonlinear functions φ and ψ are not explicit, which renders the procedure difficult to use. Indeed, at each use of the procedure, one must solve the system of equations—equations 11 and 12—which is complex and time consuming. This is where our approach using the RSM becomes useful.

The Response Surface Methodology (RSM) is a set of approaches exploring the relationships between several explanatory variables and one or more response variables. The RSM gives only an

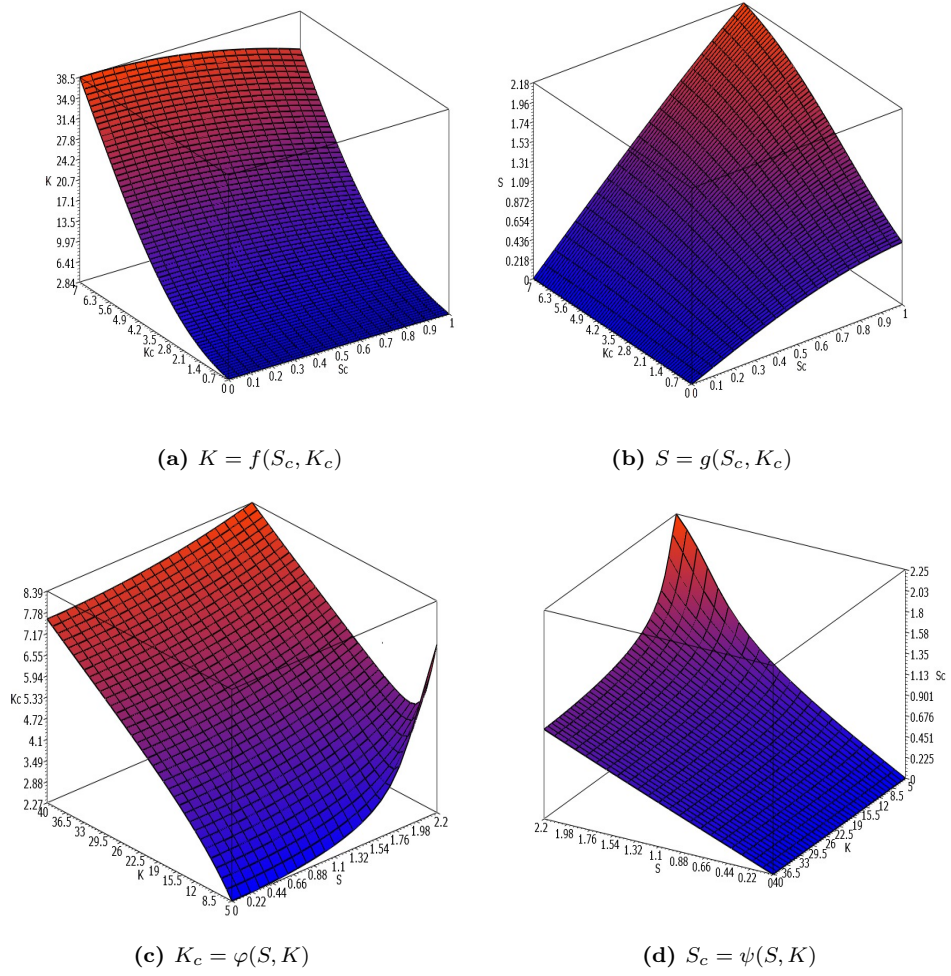


Fig. 3: Representations of the f , g , φ , and ψ functions

approximation, but it is useful because such models are easy to estimate and apply, even when little is known about the process. In practice, it means estimating a polynomial model of various functions to approximate curves or surfaces. Response surface methodology is used to optimize the parameters of a process when the function that describes it is unknown. The procedure involves fitting a function to the given data, and then using optimization techniques to obtain the optimal parameters. This procedure is usually used because it allows the development of a model that is less time consuming.

The establishment of a clear and consistent RSM optimization algorithm is important for its use as a tool in scientific applications (e.g., estimating model parameters), where results should be reproducible and derived via a clear method. All choices concerning the algorithm have to be made at the outset of an application. The main advantage of the RSM is in large-scale, time-consuming applications, such as solving equations 11 and 12. However, there is no consensus on a standard

RSM algorithm because several methods can be used.¹¹ In this work, we rely on the approaches of Sauerbrei & Royston (1999) and Royston & Sauerbrei (2008).

Technically, RSM is a stage-wise heuristic that searches through various local (sub)areas of the global area in which the simulation model is valid. We focus on the first stage, which fits first-order polynomials in the inputs, per local area. This fitting uses the ordinary least squares (OLS) approach and an ANOVA analysis.

In this study, we develop a polynomial model to obtain the two parameters S_c and K_c . The procedure implements the RSM to estimate an accurate functional form. This estimation allows us to optimize the computation time of this process. Instead of simply providing tables (such as in Maillard, 2012) of the two parameters S_c and K_c , as previous papers have done, we estimate response surface regressions. In this sense, our contribution is mainly methodological and practical, because it proposes using the RSM and makes Maillard’s correction quickly implementable. These polynomial models run much faster than the (possibly computationally expensive) numerical solver models.

Thus, a key feature of our analysis is to deal with the difficulties of standard risk modeling. In light of the recent regulations (Solvency, Basel) that followed the subprime and European debt (Greece) crises, risk measurements (and VaR and $CVaR$ estimates, in particular) are in great demand by all financial industries, as well as by regulation authorities. Yet, to date, few studies have concentrated on VaR or $CVaR$ analyses or, more generally, on risk measurement in the case of non-normally distributed asset classes. This study fills this gap in the literature by employing an approach based on Cornish–Fisher expansions. This relies on higher-order moments of returns, which results in an overall improvement in the computation of downward risk metrics, because the resulting technique proves sensitive to the characteristics of the underlying true return distribution. Therefore, this study contributes to the extant literature by proposing a new approach to risk assessment that is easily and rapidly implementable.

The remainder of the paper is organized as follows. Following a literature review in section 2, the response surface estimations are presented in section 3, with an emphasis on the adequacy of the approach. Section 4 analyzes the quality of the estimated functions. Next, an application of the proposed approach is presented in section 5. Section 6 concludes the paper.

2 Literature review and response surface methodology

Computing VaR and determining distribution quantiles have already been the subject of considerable research, following the introduction of VaR into current banking practice (for a comprehensive review of methods, see Christoffersen, 2012). For VaR estimations, key articles that examine the best methods to compute VaR include the following: Pritsker (1997), who focuses on Monte Carlo simulations, Zangari (1996) and Fallon (1996), who concentrate on Cornish–Fisher expansions, and Longin (2000), who addresses extreme value theory.

A considerable volume of research has concentrated on the best methods to compute VaR . Pichler & Selitsch (1999) compared five VaR methods in the context of portfolios and options, namely, the Johnson transformations, variance–covariance analysis, and the three Cornish–Fisher expansions of the second, fourth, and sixth orders. They concluded that a sixth-order Cornish–Fisher expansion is the best of the analyzed approaches. The work of Mina & Ulmer (1999) and Feuerverger & Wong

¹¹ Surprisingly few studies systematically compare the performances of these optimization methods.

(2000) can also be consulted. Jäschke (2001) concentrated on the properties of the Cornish–Fisher expansion, and its underlying assumptions, in the context of *VaR*, focusing particularly on the non-monotonicity of the distribution function, in which case convergence is not guaranteed.¹² Jäschke discussed how the conditions for its applicability make the Cornish–Fisher approach difficult to use in practice (points we address in this study). However, he demonstrated that when a data set obeys the required conditions, the accuracy of the Cornish–Fisher expansion is generally more than sufficient for one’s needs, in addition to being faster to implement than the other approaches. Simonato (2011) compare and document the performance of the Cornish–Fisher, Gram–Charlier, and Johnson approaches for computing value at risk and expected shortfall. His results reveal that Johnson distributions yield smaller approximation errors than the Gram–Charlier and Cornish–Fisher approaches when used with exact or estimated moments. More recently, Amédée-Manesme et al. (2015) used the Cornish–Fisher expansion and a so-called rearrangement procedure to calculate direct real estate *VaR*. They calculated a rolling *VaR* over time for returns using the UK commercial real estate IPD database, and showed how the Cornish–Fisher expansion makes it possible to adequately account for the non-normality of returns.

The conditional autoregressive value at risk (CAViaR) models developed by Engle & Manganelli (2004) provide another appealing approach to VaR estimation. CAViaR models are part of the semiparametric VaR approaches. Using an autoregressive framework, CAViaR models aim to derive the evolution of the desired quantile rather than extracting the quantile from an estimate of a complete distribution or from a volatility estimate. The approach has the advantage of allowing the shape of the conditional returns distribution to be time-varying, and for the time-variation to be different for different quantiles of the distribution. In this sense, these models are also able to deal with non-normal distribution exhibiting skewed distribution and fat-tails. Empirical evidence has shown that CAViaR models are competitive with other VaR models (see Bao et al., 2006; Yu et al., 2010) and has decent empirical performance. Even if CAViaR approaches are appealing, their implementation are challenging due to some computational difficulties of the model. In particular, quantile regressions approaches require large amount of data and numbers of parameters for implementation.

A spectrum of strategies tackling high-dimension systems appear in many different disciplines, because the high dimensionality challenge is rather universal in science and engineering fields. These strategies include parallel computing, increasing computer power, reducing design space, screening significant variables, decomposing design problems into sub-problems, mapping, and visualizing the variable/design space. These strategies tackle the difficulties caused by high dimensionality from different angles. Owing to space limitations and the fact that some of these strategies are applied in specialized areas (e.g., parallel computing and increasing computer power), this section reviews the RSM approach only.

Response surface methodology was developed by Box and collaborators in the 50s (Box & Wilson, 1992). This term was originated from the graphical perspective generated after fitness of the mathematical model, and its use has been widely adopted in texts on chemometrics. RSM consists of a group of mathematical and statistical techniques that are based on the fit of empirical models to the experimental data obtained in relation to experimental design. Toward this objective, linear or square polynomial functions are employed to describe the system studied and, consequently, to explore (modeling and displacing) experimental conditions until its optimization. Theoretical analysis and empirical tests of the RSM is reported to the books of Myers et al. (2016) and Khuri & Mukhopadhyay (2010) or the literature survey of Myers (1999).

¹² See also the chapter (by Jäschke and Jiang) of Härdle (2009) for a detailed discussion.

The RSM method dates back to Box & Wilson (1992), who used a second-degree polynomial model to represent an experiment. Box invented RSM to find the combination of inputs that minimizes the output of a real, non-simulated system. In this first attempt, they ignored constraints. There is a vast amount of research and literature on RSM. For extensive information on various aspects of RSM, we refer the reader to Box & Draper (1987), Myers (1999), Khuri & Cornell (1996), Del Castillo (2007), and Khuri & Mukhopadhyay (2010). Several surveys have drawn attention to the RSM, including Hill & Hunter (1966), Myers et al. (2004), Nwabueze (2010), and Ibrahim & Elkhidir (2011). In addition, the work of Neddermeijer et al. (2000) may be consulted for the automated optimization of stochastic simulation models using the RSM.¹³

In practice, the RSM procedure uses the method of least squares to fit quadratic response surface regression models. Response surface models are a kind of general linear model, in which attention focuses on the characteristics of the fit response function. The predicted optimal function can be found from the estimated surface if the surface is similar in shape to a simple hill or valley. If the estimated surface is more complicated, then the shape of the surface can be analyzed to indicate directions for new computations. Suppose a response variable y is measured as combinations of the values of two factor variables, x_1 and x_2 . Then, the quadratic response surface model for this variable is written as:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + \varepsilon.$$

In addition to fitting a quadratic function, the analysis includes a lack of fit test for the significance of individual factors, and a canonical analysis of the estimated response surface to examine the overall shape of the curve. If the model is adequate, then both components estimate the nominal level of the error. However, if the bias component of the error is much larger than the pure error, then this constitutes evidence that there is a significant lack of fit.

This estimation is based on a fractional polynomial regression. Regression models based on fractional polynomial functions of a continuous covariate are described by Royston & Altman (1994). Fractional polynomial regressions use an algorithm proposed by Royston & Altman (1994), Sauerbrei & Royston (1999), or Royston & Sauerbrei (2008), and are implemented using the Stata command `mfp` or using the SAS command `rsreg`. The RSM is flexible, and the recent increase in computing power allows for the easy use of a range function, such as square, cubic, log, and higher-order functions.

The RSM has been used primarily in experimental sciences, environmental and technical sciences, and in marketing. In experimental sciences, numerous experiments based on RSM have been carried out, resulting in linear and quadratic models that explain the relation between the parameters. By applying the RSM, it is possible to design experiments, build models, search for optimal conditions for desirable responses, and evaluate interactions among factors that may influence the efficiency of a treatment using a reduced number of experiments (see for instance Ahmad et al., 2007; Li et al., 2010; Prasad et al., 2011; Muhamad et al., 2013).

In environmental sciences, the RSM has been used in various ways, from trade-off analyses between variables to environmental experiments (Gunst, 1996; Isukapalli et al., 2000; Khataee, 2010). Furthermore, the RSM is widely used in technical sciences (see Bezerra et al., 2008). In the marketing field, the approach is used to catch changes that may occur in the external environment, such as changes in customers' tastes, preferences, and purchasing power, and within firms, such as technological changes or changes in a product line. The RSM approaches allow the rapid adaptation of models to extremely complex changes (see Adcroft & Mason, 2007). In this line (see Salmasnia

¹³ Note that the RSM is subject to some criticism; for example, see Giunta et al. (2006) or Khuri & Mukhopadhyay (2010).

et al. (2013) or Nath & Chattopadhyay (2007)). Finally, in operations research, the RSM has long been used in optimization techniques (see for instance Jacobson & Schruben, 1989; He et al., 2012).

3 Using the RSM to estimate the parameters S_c and K_c

The estimation process may be summarized in three steps. First, a data set of the two endogenous variables S_c and K_c is created. Second, the polynomial model and the choice of the functional form are defined. Third, the model is estimated, and then the final polynomial model is defined.

3.1 Computation of S_c and K_c

Note that φ and ψ are both implicit functions, with the two endogenous variables being unknown. In order to estimate equations 11 and 12, we require a data set containing the two endogenous variables S_c and K_c for a set of S and K of interest.

As an illustration, Table 1 reports the 20×17 values of K (in rows) and S (in columns), as presented in Maillard (2012). The grey cells correspond to the couples (S, K) that do not belong to the validity domain \mathcal{D} . For each value of K and S , the cell contains the image of $\varphi(S, K)$ in the first row (K_c) and $\psi(S, K)$ in the second row (S_c).

Table 1: S_c and K_c as a function of S and K

$K \backslash S$	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.2	1.4	1.6	1.8	2.0	2.2	
0	0	.000	.000	.002	.006	.017	.049	.145	.459	1.67	3.00	4.46	7.56	6.97	1.9	12.4	1.20	K_c
	0	.100	.203	.310	.426	.556	.711	.914	1.22	1.82	2.08	2.26	2.97	2.50	3.46	3.65	2.81	S_c
0.5	.426	.428	.432	.439	.451	.471	.501	.555	.661	.907	1.53	5.32	5.20	9.14	1.7	12.2	13.6	K_c
	0	.090	.182	.277	.376	.483	.601	.738	.909	1.14	1.47	2.63	2.26	3.23	3.45	3.64	3.81	S_c
1	.755	.757	.763	.773	.788	.810	.842	.887	.958	1.08	1.31	2.72	7.17	8.96	1.6	12.1	9.68	K_c
	0	.084	.168	.255	.345	.439	.541	.653	.781	.935	1.14	1.71	2.96	3.22	3.43	3.63	2.73	S_c
1.5	1.03	1.03	1.03	1.05	1.06	1.09	1.12	1.16	1.22	1.31	1.44	2.16	3.93	5.61	1.4	11.9	13.3	K_c
	0	.079	.159	.240	.323	.410	.501	.599	.707	.830	.976	1.41	1.92	2.22	3.42	3.62	3.79	S_c
2	1.26	1.26	1.27	1.28	1.30	1.32	1.35	1.39	1.45	1.52	1.62	2.03	3.28	5.07	6.61	11.7	13.2	K_c
	0	.075	.151	.228	.306	.388	.472	.562	.658	.764	.883	1.20	1.69	2.09	2.33	3.61	3.78	S_c
2.5	1.47	1.47	1.48	1.49	1.51	1.53	1.56	1.60	1.65	1.71	1.80	2.09	2.85	4.50	6.16	11.6	13.0	K_c
	0	.072	.145	.218	.293	.370	.405	.533	.621	.716	.821	1.08	1.47	1.93	2.23	3.60	3.77	S_c
3	1.65	1.66	1.66	1.67	1.69	1.72	1.75	1.78	1.83	1.89	1.97	2.20	2.70	3.96	5.69	7.21	12.9	K_c
	0	.070	.140	.210	.282	.356	.432	.510	.593	.681	.775	.997	1.30	1.75	2.12	2.36	3.76	S_c
3.5	1.82	1.83	1.83	1.85	1.86	1.89	1.91	1.95	2.00	2.05	2.12	2.32	2.70	3.57	5.19	6.81	12.7	K_c
	0	.068	.135	.204	.273	.344	.417	.492	.57	.652	.740	.939	1.20	1.57	1.99	2.27	3.75	S_c
4	1.98	1.98	1.99	2.00	2.02	2.04	2.07	2.11	2.15	2.20	2.27	2.45	2.75	3.37	4.71	6.38	7.87	K_c
	0	.066	.132	.198	.265	.334	.404	.476	.551	.629	.711	.894	1.12	1.43	1.84	2.18	2.41	S_c
4.5	2.13	2.13	2.14	2.15	2.17	2.19	2.22	2.25	2.29	2.35	2.41	2.57	2.83	3.31	4.33	5.95	7.51	K_c
	0	.064	.128	.193	.259	.325	.393	.463	.534	.609	.687	.858	1.06	1.32	1.69	2.07	2.33	S_c
5	2.27	2.27	2.28	2.29	2.31	2.33	2.36	2.39	2.43	2.48	2.54	2.69	2.92	3.31	4.08	5.52	7.13	K_c
	0	.063	.125	.189	.253	.317	.383	.451	.52	.592	.666	.828	1.01	1.25	1.56	1.95	2.25	S_c
6	2.53	2.53	2.55	2.56	2.58	2.61	2.64	2.68	2.73	2.78	2.92	3.11	3.41	3.90	4.84	6.35		K_c
	0	.060	.121	.181	.242	.304	.367	.431	.497	.564	.633	.781	.946	1.14	1.38	1.71	2.07	S_c
7	2.76	2.76	2.77	2.78	2.80	2.82	2.84	2.87	2.91	2.95	3.00	3.13	3.30	3.55	3.92	4.54	5.67	K_c
	0	.058	.116	.175	.234	.294	.354	.415	.478	.542	.607	.745	.896	1.07	1.27	1.53	1.86	S_c
8	2.98	2.98	2.99	3.00	3.01	3.03	3.06	3.09	3.12	3.16	3.21	3.33	3.49	3.70	4.00	4.47	5.25	K_c
	0	.057	.113	.170	.227	.285	.343	.402	.462	.523	.586	.717	.857	1.01	1.19	1.40	1.68	S_c
9	3.18	3.18	3.19	3.20	3.22	3.24	3.26	3.29	3.32	3.36	3.41	3.52	3.67	3.86	4.12	4.50	5.08	K_c
	0	.055	.110	.166	.221	.277	.334	.391	.449	.508	.568	.693	.826	.970	1.13	1.32	1.55	S_c
10	3.37	3.38	3.38	3.39	3.41	3.43	3.45	3.48	3.51	3.55	3.59	3.70	3.84	4.02	4.25	4.57	5.03	K_c
	0	.054	.108	.162	.216	.271	.326	.382	.438	.495	.553	.673	.800	.936	1.08	1.25	1.45	S_c
15	4.22	4.23	4.23	4.24	4.25	4.27	4.29	4.32	4.35	4.38	4.42	4.51	4.62	4.76	4.93	5.14	5.40	K_c
	0	.049	.099	.148	.198	.248	.298	.349	.400	.451	.503	.608	.717	.829	.948	1.07	1.21	S_c
20	4.96	4.96	4.97	4.98	4.99	5.01	5.03	5.05	5.08	5.11	5.14	5.23	5.33	5.45	5.59	5.76	5.96	K_c
	0	.047	.094	.141	.187	.235	.282	.329	.377	.425	.473	.571	.671	.773	.878	.987	1.10	S_c
25	5.64	5.64	5.65	5.66	5.67	5.69	5.70	5.73	5.75	5.78	5.81	5.89	5.99	6.10	6.23	6.38	6.55	K_c
	0	.045	.090	.135	.181	.226	.272	.317	.363	.409	.455	.548	.643	.739	.837	.937	1.04	S_c
30	6.30	6.30	6.30	6.31	6.32	6.34	6.35	6.38	6.40	6.43	6.46	6.53	6.62	6.73	6.85	6.99	7.15	K_c
	0	.044	.088	.132	.176	.221	.265	.309	.354	.398	.443	.533	.625	.717	.810	.906	1.00	S_c

We create a data set of couples (S, K) . For each of these, using the gradient method, we estimate S_c and K_c numerically. As a robustness test, we verify, in addition to the numerical convergence of the algorithms, that $f(S_c, K_c) = S$ and $g(S_c, K_c) = K$.

3.2 Estimation of the response surface(s) for (S, K) in the validity domain \mathcal{D}

We use the response surface methodology to estimate the two reverse implicit functions φ and ψ in the domain of definition. Estimations outside the domain of definition are feasible, but require more subsets (see below), which is not the subject of this study. Therefore, this is left for future research. The functions to be estimated are:

$$K_c = \varphi(S, K) \quad \text{and} \quad S_c = \psi(S, K).$$

The methodology approximates the shape of the φ and ψ functions using a linear combination of a pre-established set of variables. In this case, we use a combination of the power and logarithm of S and K .

Using the correct functional form for the response surface regressions is crucial to obtaining useful estimates. The way the RSM approach is computed is somewhat arbitrary, because many functional

forms could potentially fit the model.¹⁴ The powers are not (usually) known, and must be estimated, together with the coefficients, from the data. The estimations involve a systematic search for the best power, or combination of powers, from the permitted set. For each possible combination, a linear regression model, as just described, is fitted, and the corresponding difference from the true model is noted. The model with the lowest difference is deemed to have the best fit, and the corresponding powers and regression coefficients constitute the final functional models (Sauerbrei et al., 2007).

Our objective here is to estimate the two following equations, where ε is a random variable, such that, $E(\varepsilon) = 0$, $V(\varepsilon) = \sigma_\varepsilon^2$. This allows us to define the following stochastic models for each random variable, K_c and S_c :

$$K_c = E(K_c|S, K) + \varepsilon_K \quad (13)$$

and

$$S_c = \text{sign}(S) \times E(S_c|S, K) + \varepsilon_S. \quad (14)$$

Considerable experimentation preceded the choice of the functional form for the regression 13 and 14. Note that the obtained functions differ depending on which polynomials, powers, and functions are used as the regressors.¹⁵ Therefore, one may wish to repeat the procedure with different choices of polynomials and functions serving as output, thus computing different estimation functions, especially if the first is near the chosen critical value. Equations 15 and 16 correspond to the deterministic parts of the models:

$$\begin{aligned} E(K_c|S, K) = & \alpha + \beta_1 S^{\frac{1}{2}} + \beta_2 K^{\frac{1}{2}} + \beta_3 S + \beta_4 K + \beta_5 S^{\frac{1}{2}} K^{\frac{1}{2}} + \beta_6 S^{\frac{3}{2}} \\ & + \beta_7 K^{\frac{3}{2}} + \beta_8 S^{\frac{1}{2}} K + \beta_9 S K^{\frac{1}{2}} + \beta_{10} S^2 + \beta_{11} K^2 + \beta_{12} S K \\ & + \beta_{13} S^{\frac{3}{2}} K^{\frac{1}{2}} + \beta_{14} S^{\frac{3}{2}} K^{\frac{1}{2}} + \beta_{15} S K^2 + \beta_{16} S^2 K + \beta_{17} S^{\frac{3}{2}} K^{\frac{3}{2}} \\ & + \beta_{18} \ln(S) \ln(K) + \beta_{19} \ln(S) K + \beta_{20} S \ln(K) + \beta_{21} S^{-1} + \beta_{22} K^{-1}. \end{aligned} \quad (15)$$

In the same way, the expected value of S_c is expressed as:

$$\begin{aligned} E(S_c|S, K) = & \delta + \gamma_1 S^{\frac{1}{2}} + \gamma_2 K^{\frac{1}{2}} + \gamma_3 S + \gamma_4 K + \gamma_5 S^{\frac{1}{2}} K^{\frac{1}{2}} + \gamma_6 S^{\frac{3}{2}} \\ & + \gamma_7 K^{\frac{3}{2}} + \gamma_8 S^{\frac{1}{2}} K + \gamma_9 S K^{\frac{1}{2}} + \gamma_{10} S^2 + \gamma_{11} K^2 + \gamma_{12} S K \\ & + \gamma_{13} S^{\frac{3}{2}} K^{\frac{1}{2}} + \gamma_{14} S^{\frac{3}{2}} K^{\frac{1}{2}} + \gamma_{15} S K^2 + \gamma_{16} S^2 K + \gamma_{17} S^{\frac{3}{2}} K^{\frac{3}{2}} \\ & + \gamma_{18} \ln(S) \ln(K) + \gamma_{19} \ln(S) K + \gamma_{20} S \ln(K) + \gamma_{21} S^{-1} + \gamma_{22} K^{-1}. \end{aligned} \quad (16)$$

The ideal (and naïve) approach would have a single response surface for all (S, K) in the validity domain, which seems unrealistic. In this case, and in order to choose a trade-off between the number of subsets and the adequacy of the model, we define five subsets of the parameters S and K in the domain of definition (the choice of the number of subsets is beyond the scope of this article). This choice is somehow ad hoc. The descriptive statistics of these subsets are displayed in Table 2.

¹⁴ Standard RSM models usually include repeated powers and log transformation.

¹⁵ Although polynomials are popular in data analyses, linear and quadratic functions are severely limited in their range of curve shapes, whereas cubic and higher-order curves often produce undesirable characteristics, such as edge effects and waves (see Sauerbrei et al., 2007).

Table 2: Descriptive statistics for the five subsets (five cases)

Cases	Moment	Observations	Mean	St. deviation	Min.	Max.
Case 1	$5 \leq K \leq 40$	1,057,340	1	.0001876	.9966196	1.001096
	$0.5 \leq S \leq 2.2$	1,057,340	1	.000486	.9926362	1.003827
Case 2	$5 \leq K \leq 40$	311,500	1	.0000597	.9992079	1.000205
	$0 < S \leq 0.5$	311,500	1	.0001378	.9976897	1.001556
Case 3	$K \leq 5$	48,281	1.000001	.0004733	.9914649	1.003484
	$S \geq 0.5$	48,281	1	.0006324	.9943166	1.008879
Case 4	$K \leq 5$	23,010	1	.0003475	.9906094	1.008038
	$0.25 \leq S < 0.5$	23,010	1	.0001057	.9989517	1.001762
Case 5	$K \leq 5$	22,834	1	.0013341	.9900169	1.061144
	$0 < S < 0.25$	22,834	1	.0012247	.9737982	1.010939

RSM can be used for the whole dataset (or for an entire surface). However to beter fit the surface—or the data behind the surface—and to obtain more acurate results, the dataset is often splited. The spliting of the dataset is common when applying RSM (as suggested by Stata or SAS guides). The split usually seeks to simplify the regression analysis. Nothing is lost in terms of the precision, you can thus estimate model coefficients. As aforesaid, it is thus a tradeoff between the number of subset and the quality of the estimation. In our case, we split the dataset (or the surface) in 5 (denoted case 1 to case 5). The splited database (or splited surface) is easier to estimate and give more accurate results. The choice of the cases 1 to 5 were chosen aften multiple trials in order to get results as accurate as possible: all parameters exhibit 3 stars (p-value ≤ 0.001 , see tables 3 and 4).

For case 1, the estimations of equations 15 and 16 for S_c and K_c are displayed in equations 17 and 18, respectively. The other cases are presented in Tables 3 and 4. All estimations are for the domain of definition (non-grey cells) of Table 1. The values of R2 are all one, which shows the reliability and adequacy of the model. In addition, note that the significance thresholds are all below 0.1% (the degree of precision is analyzed in the next section). For K_c , we obtain $\hat{K}_c = \hat{\varphi}(K, S)$:

$$\begin{aligned}
\hat{K}_c = & -5.963 + 21.52 S^{\frac{1}{2}} - 1.548 K^{\frac{1}{2}} - 26.52 S + 1.820 K + 11.08 S^{\frac{3}{2}} - 0.442 K^{\frac{3}{2}} \\
& - 2.564 S^{\frac{1}{2}} K + 5.740 S K^{\frac{1}{2}} + 0.342 S^2 + 0.0016 K^2 + 0.880 S K \\
& - 3.773 S^{\frac{3}{2}} K^{\frac{1}{2}} + 0.033 S^{\frac{1}{2}} K^{\frac{3}{2}} + 0.001 S K^2 + 0.072 S^2 K - 0.021 S^{\frac{3}{2}} K^{\frac{3}{2}} \\
& - 0.721 \ln(S) \ln(K) + 0.349 \ln(S) K + 0.366 S \ln(K) + 0.366 S^{-1} - 0.555 K^{-1}, \quad (17)
\end{aligned}$$

and for S_c , we obtain $\hat{S}_c = \hat{\psi}(K, S)$

$$\begin{aligned} \hat{S}_c = & -1.816 + 6.812 S^{\frac{1}{2}} - 0.577 K^{\frac{1}{2}} - 8.635 S + 0.508 K + 4.235 S^{\frac{3}{2}} - 0.007 K^{\frac{3}{2}} \\ & - 0.848 S^{\frac{1}{2}} K + 2.671 S K^{\frac{1}{2}} - 0.097 S^2 - 0.0003 K^2 + 0.225 S K \\ & - 1.258 S^{\frac{3}{2}} K^{\frac{1}{2}} + 0.019 S^{\frac{1}{2}} K^{\frac{3}{2}} + 0.0002 S K^2 + 0.025 S^2 K - 0.0067 S^{\frac{3}{2}} K^{\frac{3}{2}} \\ & - 0.105 \ln(S) \ln(K) + 0.098 \ln(S) K - 0.845 S \ln(K) + 0.134 S^{-1} - 0.416 K^{-1}. \end{aligned} \quad (18)$$

Table 3: K_c Response surface estimator according to the 5 subsets

	Case 1	Case 2	Case 3	Case 4	Case 5
	$0.5 \leq S \leq 2.2$	$0 < S \leq 0.5$	$S \geq 0.5$	$0.25 \leq S < 0.5$	$0 < S < 0.25$
	$5 \leq K \leq 40$	$5 \leq K \leq 40$	$K \leq 5$	$K \leq 5$	$K \leq 5$
contant	-5.962***	0.0832***	1.749***	-1.612***	-0.304***
$S^{\frac{1}{2}}$	21.53***	0.0451***	-	1.894***	0.743***
$K^{\frac{1}{2}}$	-1.548***	0.732***	-6.604***	1.938***	0.597***
S	-26.52***	-0.601***	3.425***	-	-1.662***
K	1.820***	0.124***	1.313***	0.273***	0.676***
$S^{\frac{1}{2}} K^{\frac{1}{2}}$	-	0.396***	7.491***	-1.018***	-1.073***
$S^{\frac{3}{2}}$	11.08***	1.261***	-11.83***	-4.220***	0.226**
$K^{\frac{3}{2}}$	-0.0443***	-0.0195***	-0.858***	-0.141***	-0.299***
$S^{\frac{1}{2}} K$	-2.564***	-0.0704***	-	-	0.490***
$SK^{\frac{1}{2}}$	5.739***	-0.528***	-	-	2.314***
S^2	0.342***	-0.198***	9.011***	2.164***	0.463***
K^2	0.00162***	0.00181***	0.141***	0.0247***	0.0432***
$S^{\frac{3}{2}} K^{\frac{1}{2}}$	-3.773***	-0.122***	-3.346***	2.786***	-0.234***
SK	0.880***	0.0836***	0.638***	-0.454***	-0.891***
$S^{\frac{1}{2}} K^{\frac{3}{2}}$	0.0328***	0.000231***	0.110***	0.0381***	-0.0254***
SK^2	0.000901***	0.0000956***	-0.124***	-0.0392***	-0.00616***
$S^2 K$	0.0717***	0.0133***	-0.642***	-0.862***	-0.272***
$S^{\frac{3}{2}} K^{\frac{3}{2}}$	-0.0216***	-0.00373***	0.499***	0.307***	0.205***
$\ln(S) \ln(K)$	-0.721***	-0.0305***	-0.517***	0.103***	0.00942***
$\ln(S) K$	0.349***	0.00290***	-0.650***	0.0341***	-0.00642***
$S \ln(K)$	0.0928***	0.240***	0.834***	-0.481***	-0.164***
S^{-1}	0.366***	-0.000296***	0.136***	0.0164***	-0.0000209***
K^{-1}	-0.555***	-0.444***	0.0989***	-0.00817***	0.00151***
N	1,057,340	311,500	48,281	23,010	22,834
R^2	1.000	1.000	1.000	1.000	1.000

* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$

Table 4: S_c Response surface estimator according to the 5 subsets

	Case 1 $0.5 \leq S \leq 2.2$ $5 \leq K \leq 40$	Case 2 $0 < S \leq 0.5$ $5 \leq K \leq 40$	Case 3 $S \geq 0.5$ $K \leq 5$	Case 4 $0.25 \leq S < 0.5$ $K \leq 5$	Case 5 $0 < S < 0.25$ $K \leq 5$
constant	-1.816***	-0.0189***	2.111***	0.172***	0.00512***
$S^{\frac{1}{2}}$	6.812***	0.161***	-	0.132***	-0.0240***
$K^{\frac{1}{2}}$	-0.577***	0.0215***	-3.498***	-0.296***	-0.00778***
S	-8.636***	0.453***	-2.870***	-	1.277***
K	0.508***	0.00139***	-0.123***	-0.0415***	0.00499***
$S^{\frac{1}{2}} K^{\frac{1}{2}}$	-	-0.0862***	3.836***	0.346***	0.0386***
$S^{\frac{3}{2}}$	4.235***	0.326***	2.956***	1.491***	-0.114***
$K^{\frac{3}{2}}$	-0.00685***	-0.00000851***	-0.162***	-0.0327***	-0.000479***
$S^{\frac{1}{2}} K$	-0.848***	-0.00168***	-	-	-0.0336***
$SK^{\frac{1}{2}}$	2.671***	0.230***	-	-	-0.483***
S^2	-0.0969***	-0.0136***	2.008***	0.134***	0.265***
K^2	-0.000304***	0.00000232***	0.0370***	0.00278***	-0.0000520***
$S^{\frac{3}{2}} K^{\frac{1}{2}}$	-1.259***	-0.129***	-4.884***	-1.330***	-0.0857***
SK	0.226***	-0.000326***	1.720***	0.249***	0.109***
$S^{\frac{1}{2}} K^{\frac{3}{2}}$	0.0191***	-0.000151***	-0.153***	0.0333***	0.00708***
SK^2	0.000196***	0.0000493***	-0.00138	-0.00129***	-0.00487***
$S^2 K$	0.0249***	0.00662***	0.239***	0.205***	-0.0332***
$S^{\frac{3}{2}} K^{\frac{3}{2}}$	-0.00666***	-0.000649***	-0.0883***	-0.0597***	0.0161***
$\ln(S) \ln(K)$	-0.105***	0.00396***	-0.227***	-0.0109***	-0.000270***
$\ln(S) K$	0.0987***	0.000457***	-0.436***	-0.0507***	0.000262***
$S \ln(K)$	-0.845***	-0.221***	0.700***	0.114***	0.0513***
S^{-1}	0.135***	0.000228***	-0.0739***	-0.00419***	0.000000429***
K^{-1}	-0.416***	-0.0250***	0.0414***	0.00152***	0.000110***
N	1,057,340	311,500	48,281	23,010	22,834
R^2	1.000	1.000	1.000	1.000	1.000

* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$

Table 3 and 4 present the coefficients for all the 5 subsets for the corrected kurtosis (K_c) equation and the corrected skewness (S_c) equation respectively. Indeed, if equations 15 and 16 present the estimation for the case 1, these two equations are only valid for the set of parameters $0.5 \leq S \leq 2.2$ and $5 \leq K \leq 40$. The cases 2 to 5 are presented in the tables 3 and 4. The tables present the coefficients of the equations for all the cases estimated by response surface analysis. 10 equations can thus be derived from these two tables (5 for K_c and 5 for S_c). One may also noticed that all the parameters are significant with p-values below 0.001.

4 Quality of the fitted model

The adequacy of the models is determined using a model analysis, lack-of-fit test, and R2 (coefficient of determination) analysis, as described in Lee et al. (2000), Weng et al. (2001), and MacKinnon (2010). The lack of fit is a measure of the failure of a model to represent data in the experimental domain, where points were not included in the regression, or variations in the models cannot be accounted for by random error (Montgomery, 2001) (automated in most software). If there is a significant lack of fit, as indicated by a low probability value, the response predictor is discarded. In our case, we present the final results directly.

A simple, but relevant way of checking the quality of the estimation is to use the following relationships, obtained in the case of a perfect estimation:

$$f(\hat{K}_c, \hat{S}_c) = f(\hat{\varphi}(K, S), \hat{\psi}(K, S)) = K \quad (19)$$

and

$$g(\hat{K}_c, \hat{S}_c) = g(\hat{\varphi}(K, S), \hat{\psi}(K, S)) = S. \quad (20)$$

Considering the kurtosis, the lower the spread between K and $f(\hat{\varphi}(K, S), \hat{\psi}(K, S))$, the higher is the quality of the estimation. We define the relative error on the kurtosis as:

$$\text{Err}(K) = f(\hat{\varphi}(K, S), \hat{\psi}(K, S)) / K, \quad (21)$$

and the relative error on the skewness as:

$$\text{Err}(S) = g(\hat{\varphi}(K, S), \hat{\psi}(K, S)) / S. \quad (22)$$

To confirm the quality of our estimation, we compute eight graphs (scatter plots and histograms) for all subsets. Note that only the graphs for case 1 are presented in Figure 4, but all are available in the online appendix (see appendix C).

Figure 4 shows the errors graphically. As underlined by Figures 4a and 4b, we have a “good” global estimation (because we have a nearly 45 degree line). The estimation is somehow better for the kurtosis. The histograms (Figures 4c and 4d) on the second line reinforce these results, indicating that 99% of the errors on K_c are less than 1% and less than 2%, respectively, considering S_c . This conditional analysis of $\text{Err}(K)$ and $\text{Err}(S)$, based on the values of both S and K , is confirmed by Figures 4e, 4f, 4g, and 4h. The two last lines show the spread of the error as a function of S and K . By construction, the spread on the y -axis of these four graphs is the same as that on the x -axis of the corresponding histograms. Note that in these four situations, the worst estimation is plotted in the lowest values of S or K . For instance, considering the kurtosis, we observe that higher positive errors (> 1) arise when K is around 10. Nevertheless, the errors for S and K are extremely low

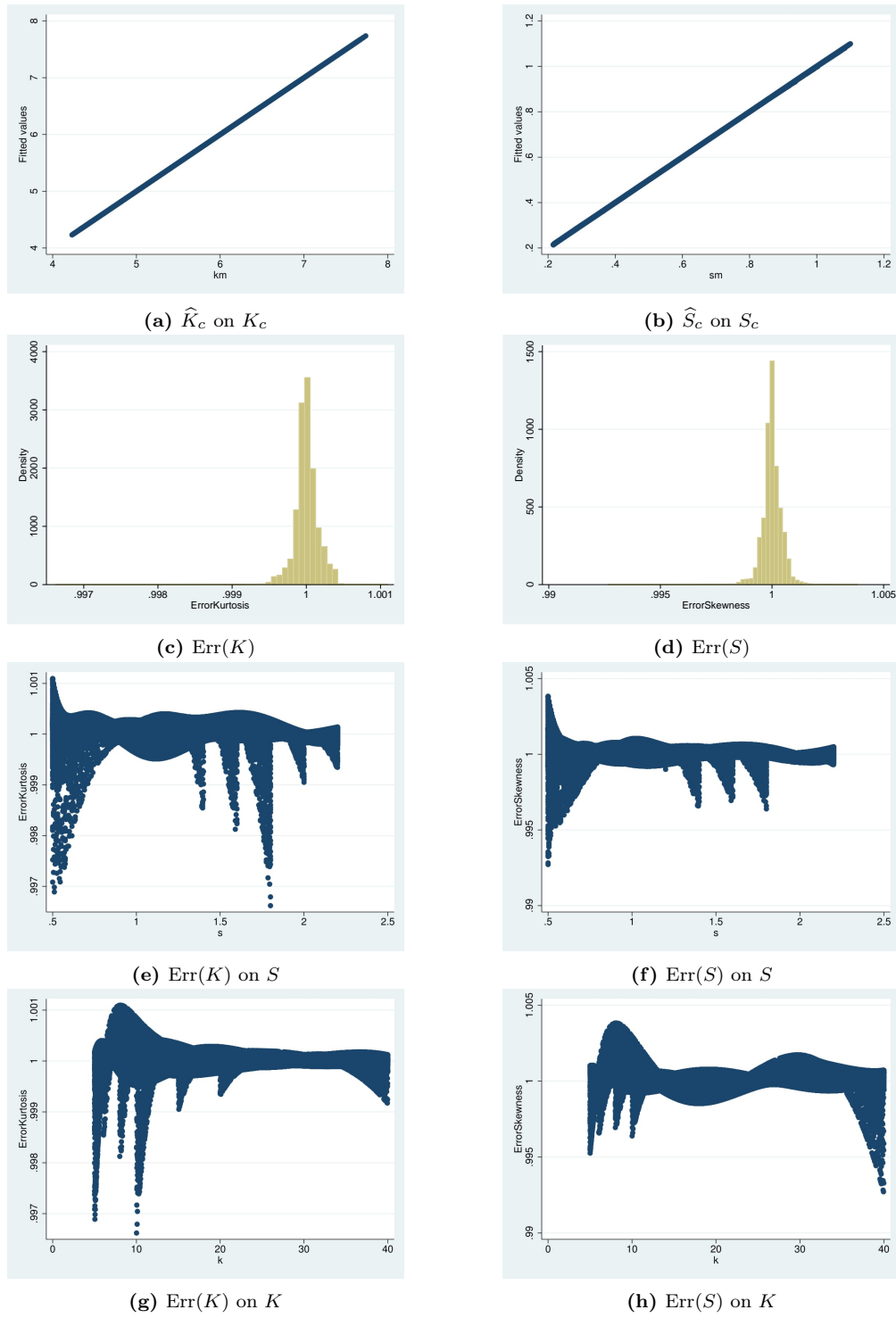


Fig. 4: Errors analysis for Case 1: $0.5 \leq S \leq 2.2$, $5 \leq K \leq 40$

(below 2%, in all cases).

This study does not aim to obtain “the best” response surface, as mentioned above, which would imply an ad hoc choice of criteria. However, this is a way of detecting where the estimation can be improved. This could also indicate points where we have to estimate two different response surfaces, rather than just one.

5 Application

We conduct two applications, one on VaR and one on $CVaR$. We use as a benchmark a theoretical distribution, namely a Student’s distribution with ν degrees of freedom. For $\nu > 4$, the expectation is equal to 0, the variance is $\nu/(\nu - 2)$, the skewness is null, and the excess of kurtosis is equal to $6/(\nu - 4)$. Table 5 underlines the usefulness of the correction, comparing the theoretical VaR with both $VaR_{CF,\alpha}$ and $VaR_{CFc,\alpha}$. The computations are based on $St(5)$ and $St(7)$. For instance, $VaR_{0.1\%}$ for $St(5)$, is equal to 5.715 (see the second line of Table 5). Using the Cornish–Fisher transformation, with $K - 3 = 6$ (S being null for a symmetric distribution), we get $VaR_{CF,0.1\%} = 6.754$. This leads to a VaR relative error of 18.20%, where the relative error is defined as the percentage error using the Cornish–Fisher VaR instead of the theoretical VaR :

$$\frac{VaR_{CF,\alpha} - VaR_{\alpha}}{VaR_{\alpha}}.$$

Using the corrected Cornish–Fisher transformation, with $Kc - 3 = 2.53$, we have $VaR_{CFc,0.1\%} = 5.863$. This leads to a corrected VaR relative error of 2.61%, defined more generally as:

$$\frac{VaR_{CFc,\alpha} - VaR_{\alpha}}{VaR_{\alpha}}.$$

In the case of $St(7)$, even if the errors between the Cornish–Fisher VaR and the true VaR are lower than those of $St(5)$, the corrected Cornish–Fisher does better, and relatively better for the smallest probabilities α (as in the previous case). For $\alpha = 0.1\%$, the relative error is around five times smaller (11.79%/2.43%), considering the correction, while it is half the size (3.31%/1.68%) with $\alpha = 2.5\%$. The corrected Cornish–Fisher has the same impact in the case of $St(7)$.

Computing the empirical mean of all VaR_{α} , for all probabilities less than α , we obtain an estimation for $CVaR_{\alpha}$. Because the non-corrected Cornish–Fisher VaR leads to higher errors for the smallest probabilities (and always with the same sign), the $CVaR$ should be poorly estimated, by construction. This is illustrated in Table 6, which shows the quality of the correction compared with the non-corrected Cornish–Fisher transformation. The last two columns correspond to the $CVaR$ relative errors. This is computed, as for VaR , by dividing the CF $CVaR$, corrected or not, by the theoretical $CVaR$. For instance, for $St(7)$, the theoretical $CVaR$ at 1% is 0.087, the non-corrected CF is 0.100, and the corrected CF is 0.089. This leads to respective relative errors of 14.40% and 3.01%:

$$\frac{CVaR_{CF,\alpha}}{CVaR_{\alpha}} = \frac{0.100}{0.087} = 1.1440, \quad \frac{CVaR_{CFc,\alpha}}{CVaR_{\alpha}} = \frac{0.089}{0.087} = 1.0301.$$

The shapes of these two errors for both $St(5)$ and $St(7)$ are represented in Figure 5.

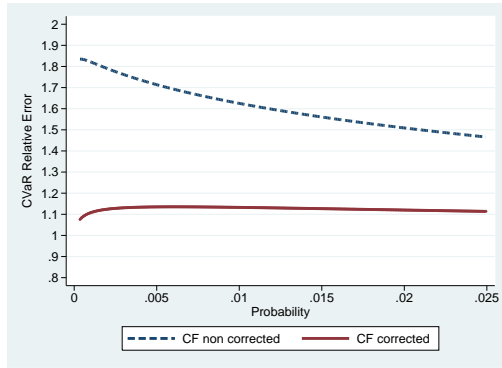
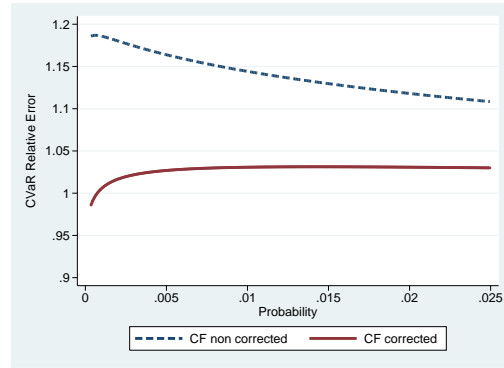
Table 5 underlines the two contributions of this paper. On one hand our methodology allows correcting the Cornish–Fisher approximation. Indeed the corrected Cornish–Fisher parameters S_c and K_c must be estimated from equations 7 and 8 which do not have solutions. The use of RSM and

Table 5: VaR computation

Student	$K - 3$	$K_c - 3$	α	VaR_α	$VaR_{CF,\alpha}$	$VaR_{CFc,\alpha}$	$\frac{VaR_{CF,\alpha}}{VaR_\alpha}$ (%)	$\frac{VaR_{CFc,\alpha}}{VaR_\alpha}$ (%)
St(5)	6	2.53	0.05%	6.515	7.755	6.605	19.03%	1.37%
			0.1%	5.715	6.754	5.863	18.20%	2.61%
			0.5%	4.149	4.710	4.303	13.51%	3.71%
			1.0%	3.551	3.917	3.673	10.29%	3.44%
			2.5%	2.799	2.938	2.866	4.96%	2.41%
			5.0%	2.242	2.247	2.268	0.21%	1.14%
St(7)	2	1.26	0.05%	5.919	6.646	5.945	12.28%	0.43%
			0.1%	5.241	5.859	5.316	11.79%	1.43%
			0.5%	3.882	4.224	3.976	8.81%	2.42%
			1.0%	3.348	3.573	3.425	6.74%	2.31%
			2.5%	2.664	2.752	2.708	3.31%	1.68%
			5.0%	2.147	2.153	2.166	0.26%	0.85%

Table 6: $CVaR$ computation

Student	$K - 3$	$K_c - 3$	α	$CVaR_\alpha$	$CVaR_{CF,\alpha}$	$CVaR_{CFc,\alpha}$	$\frac{CVaR_{CF,\alpha}}{CVaR_\alpha}$ (%)	$\frac{CVaR_{CFc,\alpha}}{CVaR_\alpha}$ (%)
St(5)	6	2.53	0.05%	3.026	5.547	3.298	83.34%	9.02%
			0.1%	1.563	2.884	1.733	81.99%	10.92%
			0.5%	0.258	0.442	0.293	71.26%	13.51%
			1.0%	0.112	0.182	0.127	62.46%	13.28%
			2.5%	0.036	0.053	0.040	46.61%	11.40%
			5.0%	0.009	0.014	0.010	15.56%	11.11%
St(7)	2	1.26	0.05%	2.094	2.485	2.082	18.69%	-0.54%
			0.1%	1.109	1.315	1.116	18.57%	0.64%
			0.5%	0.195	0.224	0.201	16.36%	2.70%
			1.0%	0.087	0.100	0.089	14.40%	3.01%
			2.5%	0.029	0.032	0.030	10.84%	2.99%
			5.0%	0.009	0.010	0.009	11.11%	11.11%

**(a)** $CVaR$ Rel. Error for a $St(5)$, $K = 6$ **(b)** $CVaR$ Rel. Error for a $St(7)$, $K = 2$ **Fig. 5:** $CVaR$ Relative Error for Student's

therefore of the estimated equations for the parameters S_c and K_c allows quick computation of the parameters and thus easily use of the Cornish–Fisher expansion. On the other hand and following the straightforward computation of the parameters S_c and K_c , the corrected Cornish–Fisher transformation able to give more accurate estimation of VaR and $CVaR$ than normal assumption or than standard–non corrected–Cornish–Fisher approach (see Figure 5).

The major finding here is therefore that the use of the corrected Cornish–Fisher expansion allied with the introduction of the RSM for its implementation allows more accurate and more straightforward computation of VaR and $CVaR$. Unlike previous findings (see section 2) where the use of the corrected Cornish–Fisher parameters was unrealistic due to the difficulty to solve the related equations (7 and 8 in this paper) and where the normal assumption was often taken for granted, this paper show how the RSM allow a straightforward and accurate use of Cornish–Fisher expansion in finance, risk management and operational research.

6 Conclusion

The challenge of risk modeling is to adequately incorporate the distribution of returns, because the under- or over-estimation of risk can lead to high losses or to significant missed opportunities. The aim of this study is to use the Cornish–Fisher expansion correctly to compute VaR and $CVaR$, highlighting the difference between the skewness and kurtosis of the distribution and those of the transformed distribution, following Maillard (2012). Calculating this difference is complicated in practice because the underlying equations cannot be solved easily. Thus, we make it straightforward to compute and use by employing the response surface methodology (RSM).

One possible weakness of the Cornish–Fisher approach is the definition of its moments and the difference between the skewness and kurtosis of the distribution and those of the transformed distribution. Indeed, the Cornish–Fisher expansion is an expansion at the third order and, therefore, one must distinguish between the moments of the distribution and those of the transformed distribution. This correction is necessary because not calculating the required moments correctly may lead to incorrect quantile estimations. However, this limitation can be resolved by transforming the original moments. This transformation relies on a set of two equations, the resolution of which are problematic and time consuming. Here, we propose an approach using the RSM that allows direct and easy computing of the transformed skewness and kurtosis in order to accurately compute VaR and $CVaR$.

The Cornish–Fisher approach does not depend on any distributional assumptions, and so may be the preferred choice when the distributional assumptions required by other modeling approaches are likely to be violated (e.g., when the return series does not follow a normal distribution, which is assumed by numerous formulations). Similarly, using our methods, we can obtain meaningful results, despite a relative paucity of data, which would render many other approaches inappropriate. These advantages may argue for using our approach in a more general risk management and assessment context. Hence, there are good reasons for practitioners, as well as banks and insurers, to implement this method alongside other models when working in a non-normal context, or whenever data sets prove modest. In addition, the proposed approach can be used for regulatory purposes as a proxy for the true VaR or $CVaR$ when conducting control and backtesting procedures.

Finally, while we limited the use of our techniques to the computation of quantiles using the Cornish–Fisher expansion, many other financial tools (all requiring complex equations) may also profit from our approach based on the RSM. It should be possible, and potentially quite interesting,

to apply our approach to risk comparisons among these various asset classes, and then to apply this to optimal portfolio choice. Risk managers who need to develop appropriate models of risk should find a useful approach here, one yielding “internal models” applicable to many asset classes.

Although the methods used to obtain these results are quite computationally intensive, they are entirely feasible with current personal computer technology. The use of response surface regressions to obtain accurate function is valuable for two reasons. First, this approach allows one to properly use the Cornish–Fisher expansion without confusing the skewness and kurtosis of the distribution with that of the transformation. Second, it makes it possible to relatively quickly compute the quantile resulting from the corrected Cornish–Fisher expansion. Similar methods could be employed in many other cases where standard numerical methods are time consuming.

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A Appendix: Quantile Functions

The quantile function (or inverse cumulative distribution function) of the probability distribution of a random variable specifies, for a given probability, the value that the random variable will fall below, with the specified probability. In fact it is an alternative to the probability density function (pdf).

Let X be a random variable with a distribution function F , and let $\alpha \in (0, 1)$. A value of x such that $F(x) = P(X \leq x) = \alpha$ is called a quantile of order α for the distribution. Then, we can define the quantile function by:

$$q_\alpha(X) \equiv F^{-1}(\alpha) = \inf \{x \in \mathbb{R} : F(x) \geq \alpha\}, \alpha \in (0, 1).$$

Thus, the quantile function $q_\alpha(X)$ yields the value that the random variable of the given distribution will fail to exceed, with probability α .

B Appendix: The Cornish–Fisher procedure

The Cornish–Fisher expansion is a useful tool for quantile estimations. For any $\alpha \in (0, 1)$, the upper α -th quantile of F_n is defined by $q_n(\alpha) = \inf \{x : F_n(x) \geq \alpha\}$, where F_n denotes the cumulative distribution function of $\xi_n = (\sqrt{n}/\sigma)(\bar{X} - \mu)$, and \bar{X} is the sample mean of independent and identically distributed observations X_1, \dots, X_n . If z_α denotes the upper α -th quantile of $N(0, 1)$, then the fourth-order Cornish–Fisher expansion can be expressed as follows:

$$q_n(\alpha) = z_\alpha + \frac{1}{6\sqrt{n}}(z_\alpha^2 - 1)S + \frac{1}{24n}(z_\alpha^3 - 3z_\alpha)(K - 3) - \frac{1}{36n}(2z_\alpha^3 - 5z_\alpha)S^2 + o(n^{3/2}), \quad (23)$$

where S and K are the skewness and kurtosis of the observations X_i , respectively.

The Cornish–Fisher expansion is useful because it allows one to obtain more accurate results compared to those acquired using the central limit theorem (CLT) approximation, which is the same as z_α defined in the main text. A demonstration and example of the greater accuracy provided by the Cornish–Fisher expansion compared to the CLT approximation is reported by Chernozhukov et al. (2010).

In general, relation (23) grants a non-monotonic character to $q_n(\alpha)$, which means that the true distribution's ordering of quantiles is not preserved. Thus, the Cornish–Fisher expansion formula is valid only if the skewness and kurtosis coefficients of the distribution meet a particular constraint. This domain of validity has been studied by Maillard (2012), among others. Monotonicity requires the derivative of $z_{CF,\alpha}$, relative to z_α , to be non-negative. This leads to the following constraint, which implicitly defines the domain of validity (D) of the Cornish–Fisher expansion:

$$\frac{S^2}{9} - 4 \left(\frac{K-3}{8} - \frac{S^2}{6} \right) \left(1 - \frac{K-3}{8} - \frac{5S^2}{36} \right) \leq 0. \quad (24)$$

In practice, this constraint is rarely considered, because S and K are generally considered to be small in finance applications.

C Online appendix - Quality of the estimation results for case 2 to case 5

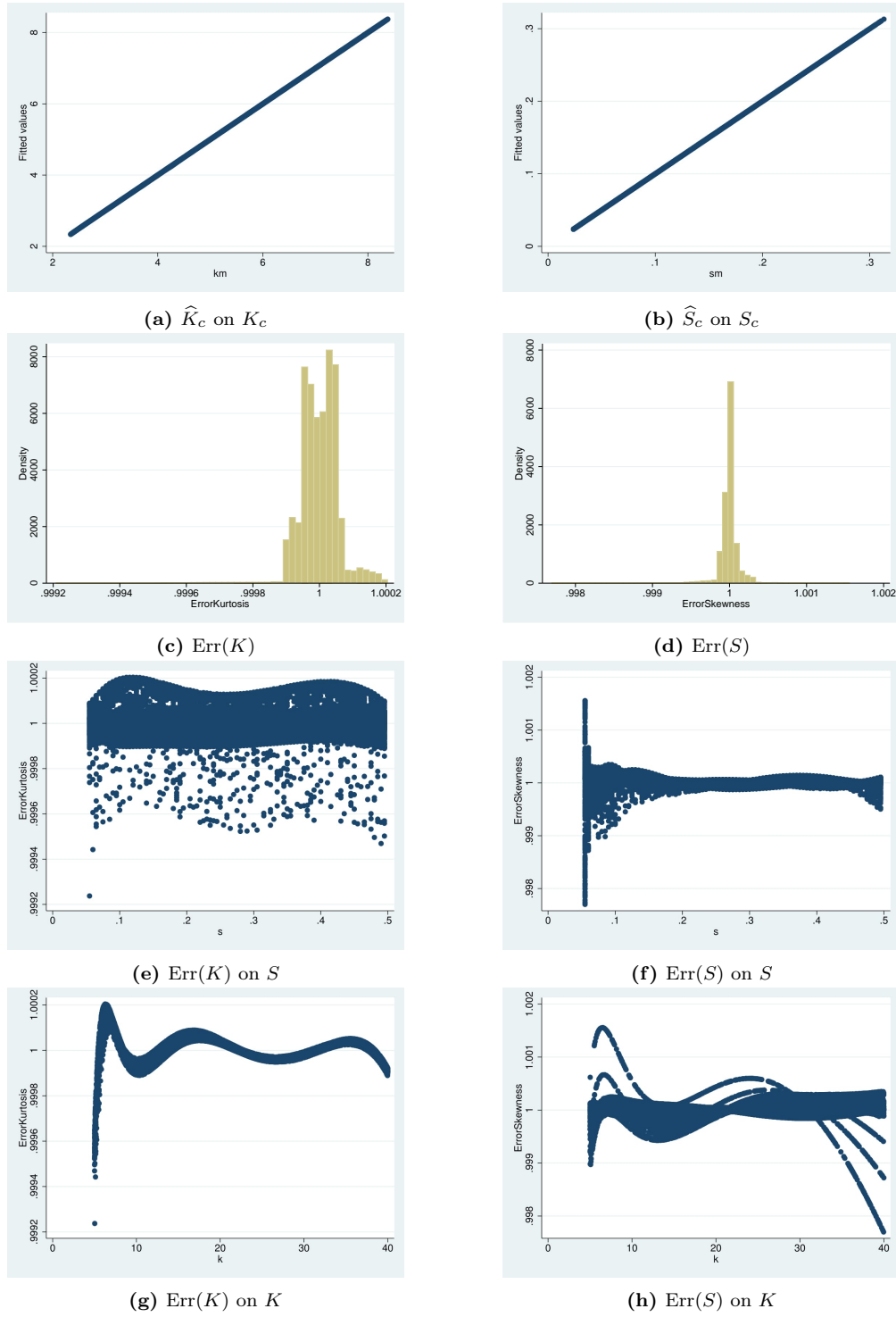


Fig. 6: Errors analysis for Case 2: $0 < S \leq 0.5$, $5 \leq K \leq 40$

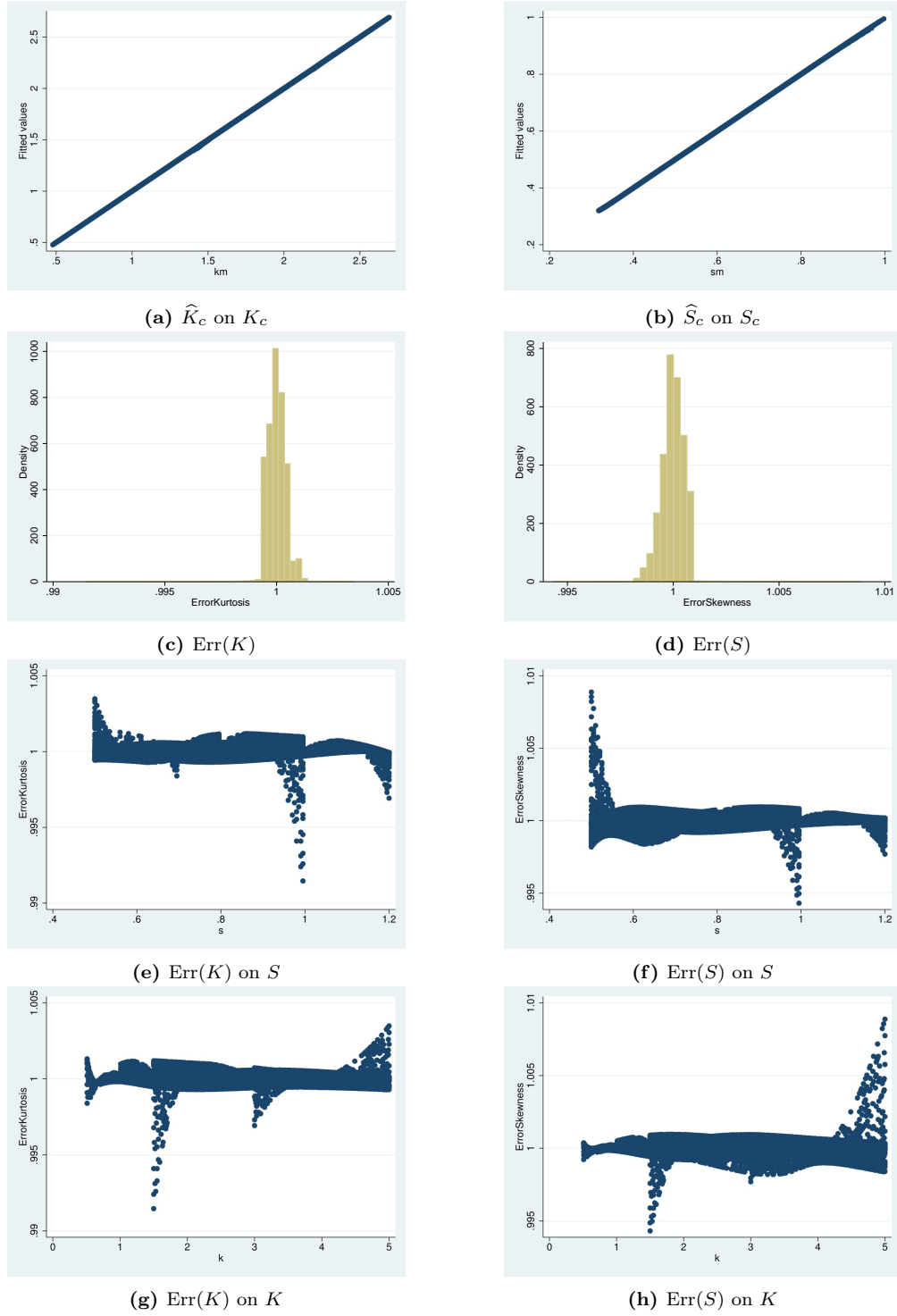


Fig. 7: Errors analysis for Case 3: $S \geq 0.5$, $K \leq 5$

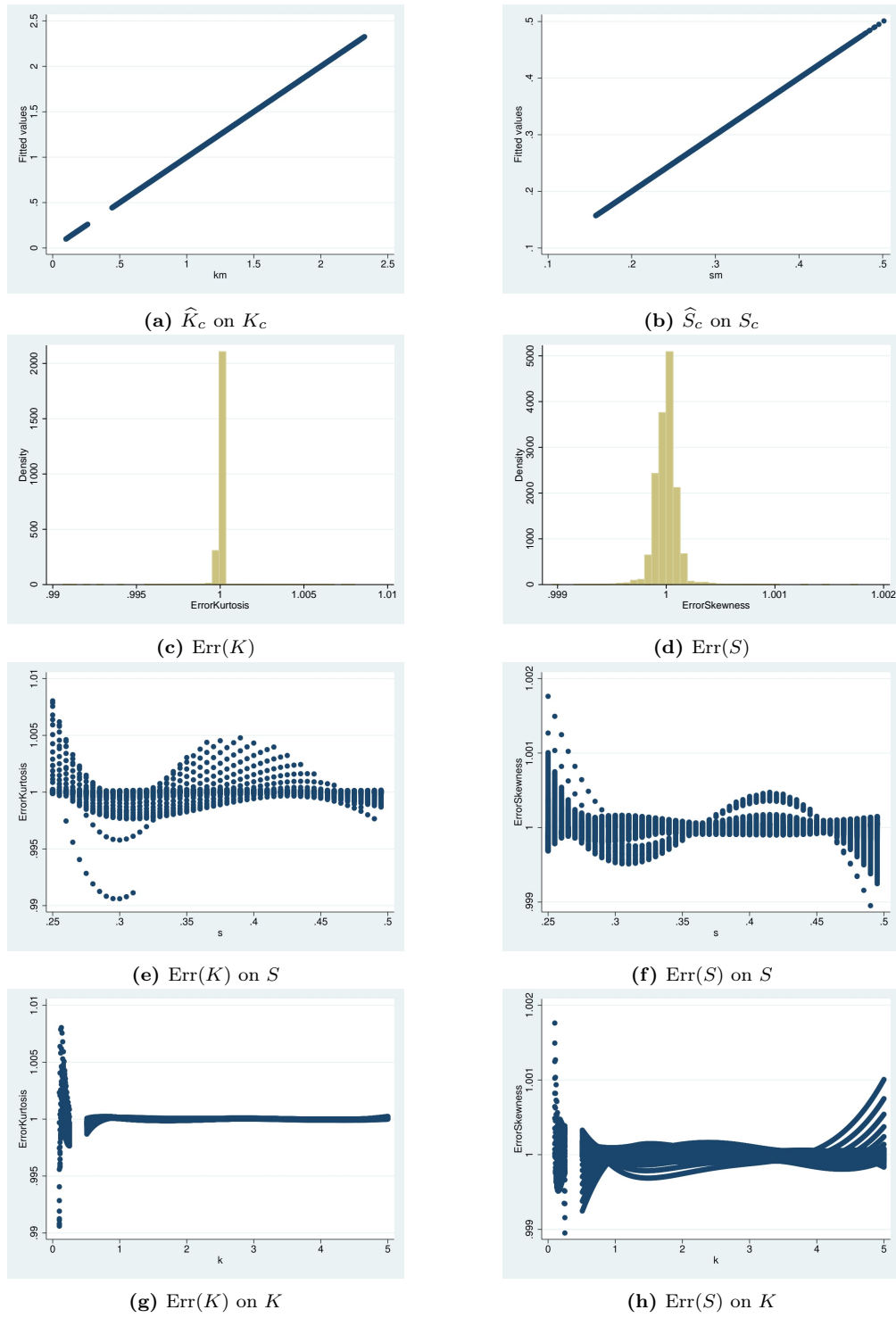


Fig. 8: Errors analysis for Case 4: $0.25 \leq S < 0.5$, $K \leq 5$

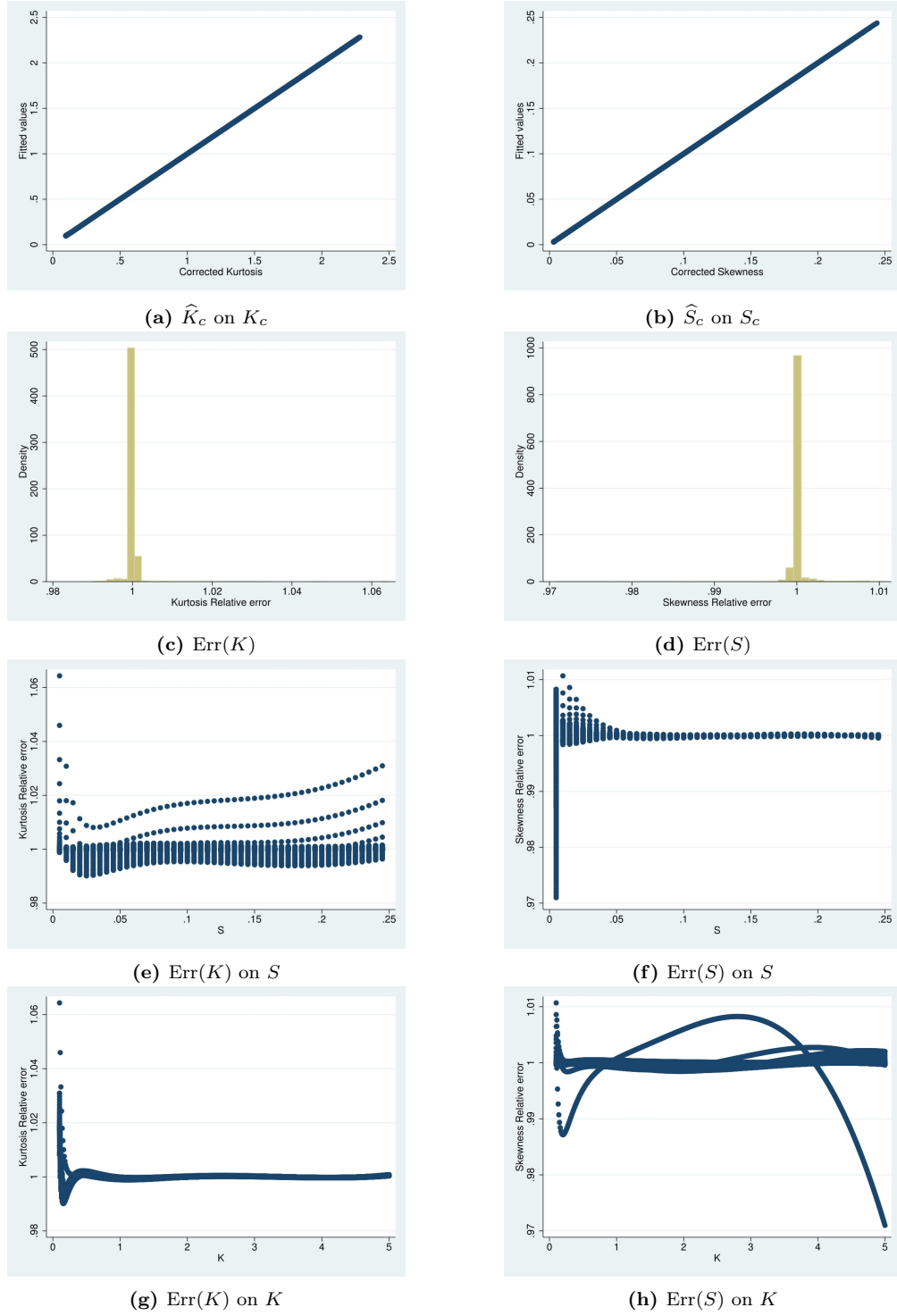


Fig. 9: Errors analysis for Case 5: $0 < S < 0.25$, $K \leq 5$