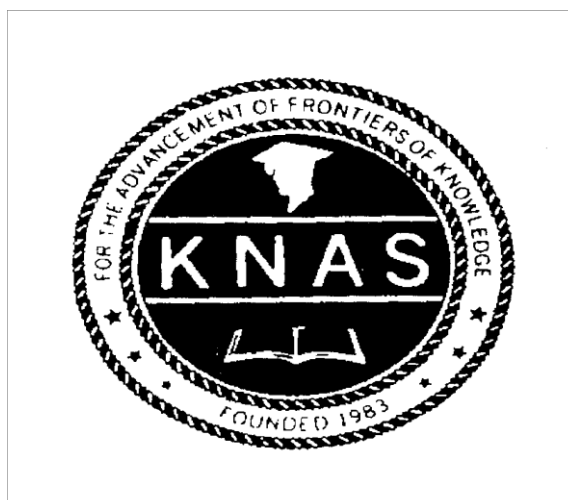


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Copula Modelling of Insurance Risks with a Hierarchical Dependence Structure

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ABSTRACT: *Insurance companies maintain different lines of business, in their operations, as a mode of diversification to aid in reducing risks of encountering ruin. These could be the portfolio profiles for the companies. The dependence structure of these lines of business cannot be ignored especially in rate making, Economic Capital assessment and in Enterprise Risk Management. However, in the real world one would find that risks are more heterogeneous than homogeneous - a problem that can be solved by breaking down the risks into a number of homogeneous categories so that we can now think of the lines of business to contain sub-classes which are homogeneous. The lines depict a hierarchical structure from the sub-classes to the main lines of business up to the portfolio level and their dependence structure is studied here by the hierarchical copulas. The less dependent sub-classes are managed in the same departments as this creates a diversified environment for tackling unsystematic risks. Moving up the hierarchy has the less dependent departments managed together and so on.*

Key words: Copula, Measures of dependence, Hierarchical Archimedean Copulas, Lines of business

INTRODUCTION

The term *copula* was first used in the work of Sklar (1959) and is derived from the Latin word *copulare*, meaning to connect or to join and has recently found an extensive acceptance in risk management, financial and insurance applications. The main purpose of copulas is to describe the interrelation of several random variables. A copula is a function that joins or couples a multivariate distribution function to univariate marginal distribution functions and so a copula is a multivariate distribution function.

Measures of dependence summarize a complicated dependence structure in a single number, in the bivariate case. The three important concepts in measuring dependence include: The classical linear correlation, rank correlation and the coefficients of tail dependence. The last two measures are general enough to give sensible measures for any dependence structure since correlation is

only a suitable measure in a special class of distributions, that is, elliptical distributions. They provide, perhaps, the best alternatives to the linear correlation coefficient as a measure of dependence for non-elliptical distributions for which the linear correlation coefficient is inappropriate and often misleading. Copulas capture these properties of the joint distribution which are invariant, that is, they remain unchanged under strictly increasing transformations of the random variables.

Frees and Valdez (1997) introduced actuaries to the concept of “copulas”, as a tool for understanding relationships among multivariate outcomes. The work explores some of the practical applications, including estimation of joint life mortality and multiple decrement models and showed how to fit copulas and hence described their usefulness by pricing a reinsurance contract and estimating expenses for pre-specified losses. Motivated by the fact that most of the Economic Capital assessment models encounter difficulties when trying to incorporate the dependence of claim costs between different Lines of Business (LOBs), Faivre (2003) suggested the use of copula theory as a solution to this problem. Other useful literature include: Embrechts, *et al.* (2002), Frees and Wang (2004), Pettere and Kollo (2006), Wu *et al.* (2006), Gatzert *et al.*, (2008) and Filler *et al.* (2009). Faivre (2003) used copulas to model the overall distribution of claim costs of four-Lines of Business company. The work utilized different copulas to show that the dependence structure has a substantial impact on the Economic Capital of that firm. We now extend the study to cover Lines of Business with sub-classes.

The Copula Function

The operational definition of a copula is a multivariate distribution function defined on the unit cube $[0,1]^n$, with uniformly distributed marginals.

Definition 1 A two-dimensional copula function (or a 2-copula) is defined as a binary function $C : [0,1]^2 \rightarrow [0,1]$, which satisfies the following three properties:

1. $C(u, 0) = C(0, u) = 0$ for any $u \in [0,1]$.
 2. $C(u, 1) = C(1, u) = u$ for any $u \in [0,1]$.
 3. For all $0 \leq u_1 \leq u_2 \leq 1$ and $0 \leq v_1 \leq v_2 \leq 1$
- $$C([u_1, v_1] \times [u_2, v_2]) = C(u_2, v_2) - C(u_1, v_2) - C(u_2, v_1) + C(u_1, v_1) \geq 0. \quad (1)$$

Due to the properties 1-3, when the arguments u and v are univariate distribution functions F_1 and F_2 , the copula function $C(F_1; F_2)$ is a legitimate bivariate distribution function with marginals F_1 and F_2 . Conversely, any bivariate distribution function $H(x; y)$ with continuous marginals F_1 and F_2 admits a unique representation as a copula function:

$$C(u, v) = H(F_1^{-1}(u), F_2^{-1}(v)) \quad (2)$$

In general, an n -dimensional copula is any function $C: [0,1]^n \rightarrow [0,1]$ such that:

1. C is grounded and n -increasing
2. C has margins $C_k, k=1,2,\dots,n$, which satisfy $C_k(u) = u$ for all u in $[0,1]$.

It is also important to note that for any n -copula, $n \geq 3$, each k -dimensional margin of C is a k -copula.

Theorem (Sklar's Theorem for n -copula)

Let H be an n -dimensional distribution function with margins $F_1, \dots, F_n$. Then there exists an n -copula C such that for all $\mathbf{x}$ in $\bar{\square}^n$,

$$H(x_1, \dots, x_n) = C(F_1(x_1), \dots, F_n(x_n)). \quad (3)$$

If $F_1, \dots, F_n$ are all continuous, then C is unique; otherwise C is uniquely determined on $\text{Ran } F_1 \times \dots \times \text{Ran } F_n$ (where $\text{Ran } F_i$ refers to the range of F_i). Conversely, if C is an n -copula and $F_1, \dots, F_n$ are distribution functions, then the function H defined in (3) is an n -dimensional distribution function with margins $F_1, \dots, F_n$.

Corollary Let H be an n -dimensional distribution function with continuous margins $F_1, \dots, F_n$ and copula C . Then for any $\mathbf{u}$ in $[0,1]^n$,

$$C(u_1, \dots, u_n) = H(F_1^{-1}(u_1), \dots, F_n^{-1}(u_n)). \quad (4)$$

Fréchet–Hoeffding Copula Boundaries

A copula always lies in between certain bounds. The reason for this is the existence of some extreme cases of dependency.

Minimum copula: This is the lower bound for all copulas. It represents perfect negative dependence between variates. For n -variate copulas, the lower bound is given by

$$W(u_1, u_2, \dots, u_n) = \max_{i \in \{1, \dots, n\}} \left\{ 1 - n + \sum_{i=1}^n u_i, 0 \right\} \leq C(u_1, u_2, \dots, u_n). \quad (5)$$

Maximum copula: This is the upper bound for all copulas which represents perfect positive dependence between variates. For n -variate copulas, the upper bound is given by

$$C(u_1, u_2, \dots, u_n) = \min_{j \in \{1, \dots, n\}} u_j = M(u_1, u_2, \dots, u_n) \quad (6)$$

For all copulas $C(u_1, u_2, \dots, u_n)$,

$$W(u_1, u_2, \dots, u_n) \leq C(u_1, \dots, u_n) \leq M(u_1, \dots, u_n) \quad (7)$$

The random variables X and Y are *comonotonic* if they have the Fréchet-Heoffding upper copula. Further, they are *counter-comonotonic* if they have the Fréchet-Heoffding lower copula.

Families of Copula

Elliptical copulas

These are the copulas with an elliptical form and therefore symmetric in the tails. Important copulas in this family are the Gaussian and the Student's t -copula together with the Cauchy Copula which is a special case of the t -copula. Differentiating (4) gives the density of an elliptical copula

$$c(u_1, \dots, u_n) = \frac{f[F_1^{-1}(u_1), \dots, F_n^{-1}(u_n)]}{\prod_{i=1}^n f_i[F_i^{-1}(u_i)]} \quad (8)$$

where f is the joint PDF of the elliptical distribution, and $f_1, \dots, f_n$ are marginal density functions.

The Gaussian Copula

For 2-dimensional case, the Gaussian copula may be represented as:

$$C^{Ga}(u, v; \rho) = \Phi_{\Sigma}^2(\Phi^{-1}(u), \Phi^{-1}(v)) \\ = \int_{-\infty}^{\Phi^{-1}(u)} \int_{-\infty}^{\Phi^{-1}(v)} \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left\{-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}\right\} dx dy \quad (9)$$

where $\Phi(x)$ is the standard normal distribution function and $\Phi_{\Sigma}^2(x, y)$ is the bivariate normal distribution with zero mean and correlation ρ between the marginals, that is, Σ is a 2×2 matrix with 1 on the diagonal and ρ otherwise.

For $\rho=0$, the Gaussian copula equals the independence copula. If $\rho=1$ we obtain the comonotonicity copula, while for $\rho=-1$ the counter-comonotonicity copula is obtained. The

Gaussian copula interpolates between these three fundamental dependency structures via one simple parameter, the correlation ρ . A copula with this feature is referred to as comprehensive.

The copula of the n -variate normal distribution with covariance matrix Σ is

$$C_{\rho}^{Ga}(\mathbf{u}) = \Phi_{\rho}^n(\Phi^{-1}(u_1), \dots, \Phi^{-1}(u_n)), \quad (10)$$

where Φ_{ρ}^n denotes the joint distribution function of the n -variate standard normal distribution function with covariance matrix Σ , and Φ^{-1} denotes the inverse of the distribution function of the univariate standard normal distribution.

Gaussian copulas do not have upper tail dependence, Joe (1997). Since elliptical distributions are radially symmetric, the coefficients of upper and lower tail dependence are equal. Hence Gaussian copulas do not have lower tail dependence either.

The t - Copula

In the bivariate case the t-copula expression can be represented as:

$$\begin{aligned} C^t(u, v; \rho, \nu) &= t_{\rho, \nu}^2(t_{\nu}^{-1}(u), t_{\nu}^{-1}(v)) \\ &= \int_{-\infty}^{t_{\nu}^{-1}(u)} \int_{-\infty}^{t_{\nu}^{-1}(v)} \frac{1}{2\pi\sqrt{1-\rho_{12}^2}} \frac{1}{\left\{1 + \frac{x^2 - \rho_{12}xy + y^2}{\nu(1-\rho_{12}^2)}\right\}^{1+\nu/2}} dx dy \end{aligned} \quad (11)$$

where $t_{\nu}(x)$ is t -distribution with ν degrees of freedom and $t_{\rho, \nu}^2(x, y)$ is bivariate t -distribution with correlation ρ .

If $(X_1, X_2)^T$ has a standard bivariate t -distribution with ν degrees of freedom and linear correlation matrix ρ , then $X_2|X_1 = x$ is t -distributed with $\nu + 1$ degrees of freedom and

$$E(X_2|X_1 = x) = \rho_{12}x, \quad Var(X_2|X_1 = x) = \left(\frac{\nu + x^2}{\nu + 1}\right)(1 - \rho_{12}^2). \quad (12)$$

This result can be used to show that the t-copula has upper tail dependence (and because of radial symmetry) equal lower tail dependence:

$$\lambda_U = 2 \lim_{x \rightarrow \infty} P(X_2 > x | X_1 = x) = 2 \bar{t}_{\nu+1} \left(\sqrt{\nu+1} \sqrt{1-\rho_{12}} / \sqrt{1+\rho_{12}} \right) \quad (13)$$

The quantity λ_U ranges between -1 and 1, Coles *et al.* (1999). The following graphicals were plotted from simulated data in order to help us visualise the characteristics of the Normal Copula and the t-Copula.

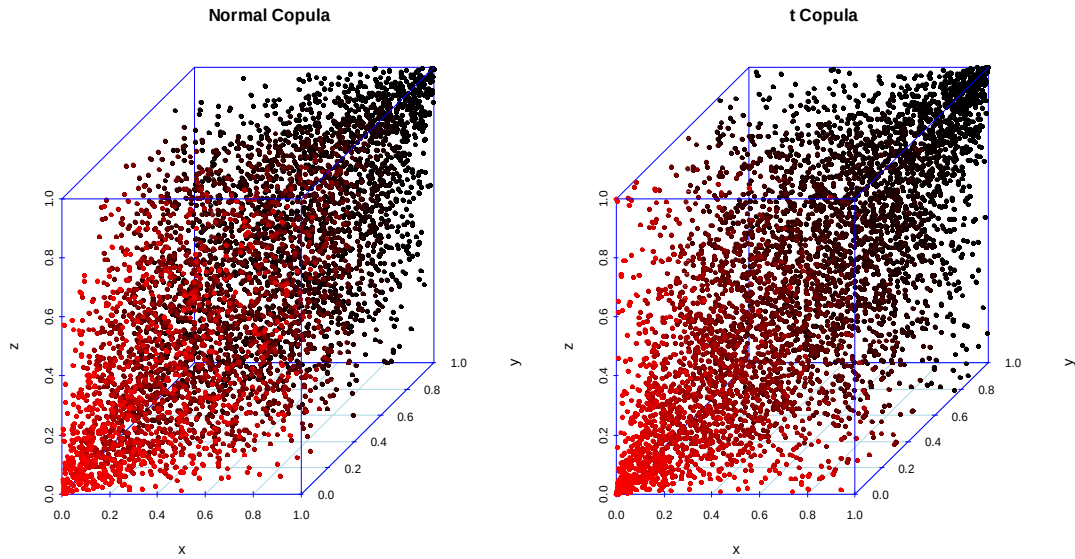


Figure 1a: Scatter plots of 5000 random numbers from a normal copula and a t-copula. Both have a dependence parameter of 0.5 with the t-distribution having 3 df. Notice the dependence at the tails of each distribution. The t-distribution has a more flexible structure and an increasing dfs, the scatter plot will approach the normal copula as displayed Figure 1b:

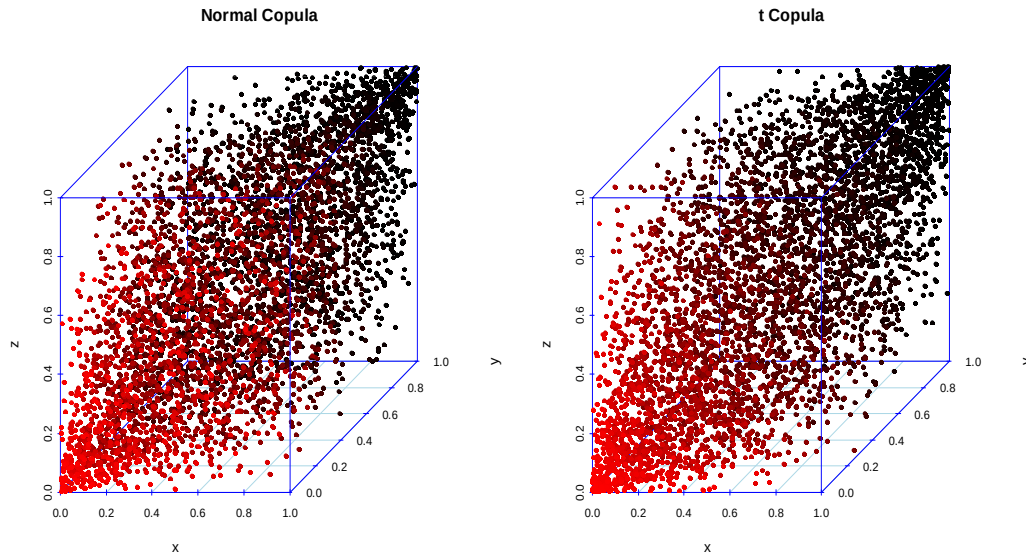


Figure 1b: Scatter plots of 5000 random numbers from a normal copula and a t-copula. Both have a dependence parameter of 0.5 with the t-distribution having 15 df.

The Cauchy Copula

This is a special case of the Student-t copula where the degrees of freedom is $\nu = 1$. The copula generated by a multivariate Cauchy distribution with linear correlation matrix Σ is given by:

$$C(u_1, \dots, u_n) = T_1(t_1^{-1}(u_1), \dots, t_1^{-1}(u_n)) \quad (14)$$

where T_1 is the joint distribution function of a standard Cauchy random vector expressed as

$$T_1(x_1, \dots, x_n) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right) \pi^{n/2} \sqrt{|\Sigma|}} \int_{-\infty}^{x_n} \int_{-\infty}^{x_{n-1}} \dots \int_{-\infty}^{x_1} (1 + z^T \Sigma^{-1} z)^{-\frac{(n+1)}{2}} dz_1 \dots dz_n \quad (15)$$

and $t_1^{-1}(\cdot)$ is the inverse of a standard Cauchy distribution with $t_1(z) = \int_{-\infty}^z \frac{1}{\pi} \cdot \left(\frac{1}{1+\omega}\right)^2 d\omega$. Due to its relationship with the Student-t copulas, we deduce that Cauchy copulas also have non-zero tail dependence. This can be seen from Figure 2 for the Cauchy copula in relation to Figure 1a for the t-copula plate.

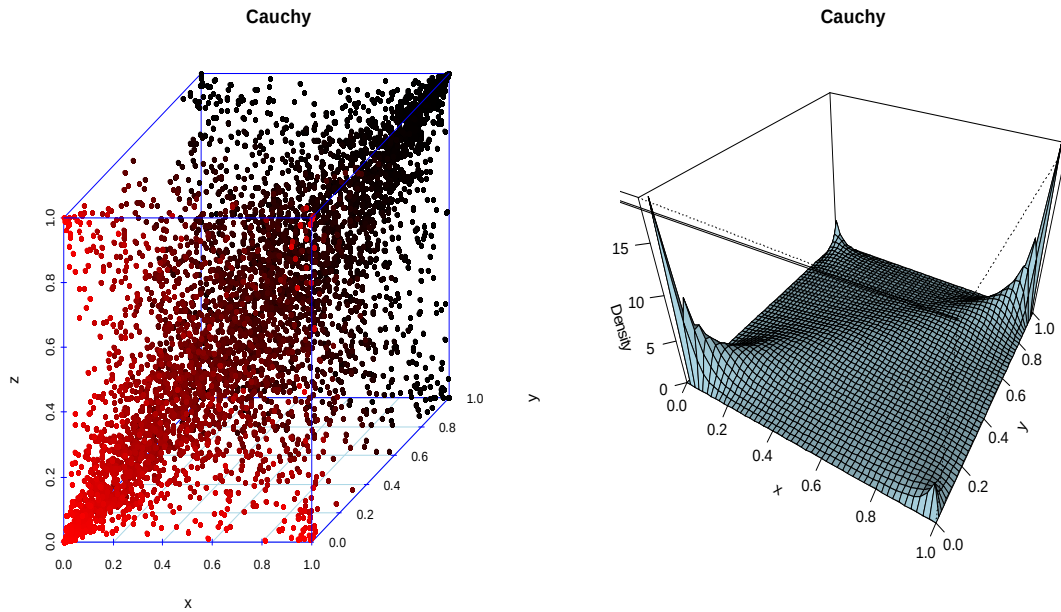


Figure 2: Scatter and perspective plots for Cauchy distributed random variables with a dependence of 0.5.

Archimedean copulas

Archimedean copulas are widely applied, because they are not difficult to construct. In comparison to Elliptical copulas, Archimedean copulas have only one dependency parameter (instead of a dependency matrix) and have many different forms.

Definition 2 Let $\varphi : [0, 1] \rightarrow [0, \infty]$ be a continuous, strictly decreasing and convex function such that $\varphi(1) = 0$ and $\varphi(0) = \infty$.

The function φ has an inverse $\varphi^{-1} : [0, \infty] \rightarrow [0, 1]$ with the same properties like φ , except that $\varphi^{-1}(0) = 1$ and $\varphi^{-1}(\infty) = 0$.

Definition 3 The function $C : [0, 1]^n \rightarrow [0, 1]$ defined by

$$C(u_1, \dots, u_n) = \varphi^{-1}(\varphi(u_1) + \dots + \varphi(u_n)) \quad (16)$$

is called n -dimensional Archimedean copula IFF φ^{-1} is completely monotonic on $[0, \infty)$, that is

$$(-1)^k \frac{\partial^k}{\partial u^k} \varphi^{-1}(u) \geq 0 \quad \text{for } k \in \mathbb{N} \quad (17)$$

The function φ is called the generator of the copula. We assume that the generator φ has only one parameter, denoted as θ .

If $\varphi(0) = \infty$ we say that φ is a strict generator, and the copula is said to be a strict Archimedean copula. One particularly simple form of a n -dimensional *Archimedean* copula is

$$H(x_1, x_2, \dots, x_n) = \varphi^{-1} \left(\sum_{i=1}^n \varphi(F_i(x_i)) \right) \quad (18)$$

where φ is known as a *generator function* and $F_i(X_i)$ (for $i = 1, \dots, n$) is the marginal distribution of the continuous random variable X_i . Any generator function which satisfies the properties below is the basis for a valid copula:

$$\varphi(1) = 0; \quad \lim_{x \rightarrow 0} \varphi(x) = \infty; \quad \varphi'(x) < 0; \quad \varphi''(x) > 0. \quad (19)$$

Product copula: Also called the independent copula, this copula has no dependence between variates. Its density function is unity everywhere.

$$\varphi(x) = -\ln(x); \quad H(x, y) = F(x)G(y) \quad (20)$$

A simple generalisation of the multivariate Archimedean copula can be found in Breymann *et al.* (2003) and Whelan (2004). The copula for the n -dimensional case requires $n - 1$ generators $\varphi_1, \dots, \varphi_{n-1}$,

$$\begin{aligned} C(u_1, \dots, u_n) \\ = \varphi_{n-1}^{-1}(\varphi_{n-1} \circ \varphi_{n-2}^{-1}[\dots(\varphi_2 \circ \varphi_1^{-1}[\varphi_1(u_1) + \varphi_1(u_2) + \varphi_2(u_3)) \\ + \dots + \varphi_{n-2}(u_{n-2})] + \varphi_{n-1}(u_n)) \end{aligned} \quad (21)$$

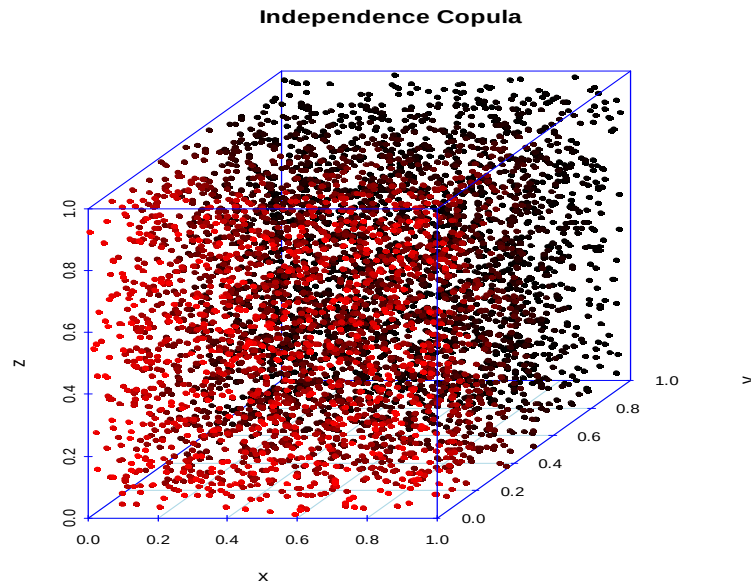


Figure 3: Scatter plot for the independence copula

This is referred to as fully nested, since a higher dimensional copula is obtained by adding one dimension step by step as shown in Figure 4:

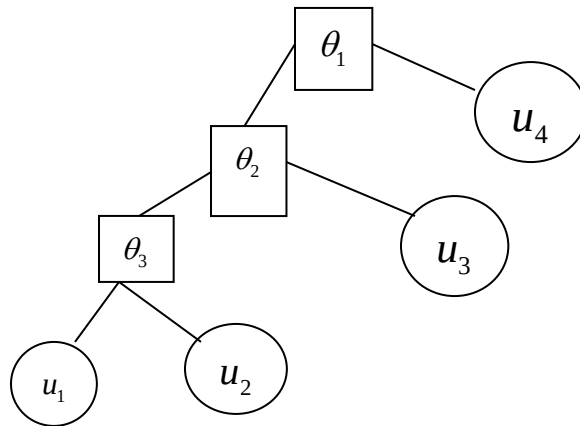


Figure 4: Fully nested copula with a dimension of $n = 4$

The second generalisation method of multivariate Archimedean copulas is more flexible than the fully nested one. It is a mixture of exchangeable and fully nested copulas and is referred to as partially nested. The lowest dimension in which a copula from this class exists is $n = 4$, and the copula is

$$C(u_1, \dots, u_4) = \varphi^{-1} \left(\varphi \circ \varphi_{12}^{-1} [\varphi_{12}(u_1) + \varphi_{12}(u_2)] + \varphi \circ \varphi_{34}^{-1} [\varphi_{34}(u_3) + \varphi_{34}(u_4)] \right) \quad (22)$$

with three generators φ, φ_{12} and φ_{34} . The three often used Archimedean copulas include Clayton, Gumbel, and Frank.

The Clayton copula

The Clayton copula is an asymmetric Archimedean copula, exhibiting greater dependence in the negative tail than in the positive. This copula is given by:

$$C_\theta(u, v) = \max \left(\left[u^{-\theta} + v^{-\theta} - 1 \right]^{-\frac{1}{\theta}}, 0 \right) \quad (23)$$

And its generator is:

$$\varphi_\theta(x) = \frac{1}{\theta} (x^{-\theta} - 1) \quad \text{where, } \theta \in [-1, \infty) \setminus \{0\} \quad (24)$$

The Gumbel copula

The Gumbel copula (also referred to as the Gumbel-Hougaard copula) is an asymmetric Archimedean copula, exhibiting greater dependence in the positive tail than in the negative. This copula is given by:

$$C_\theta(u, v) = \exp \left\{ - \left[(-\ln u)^\theta + (-\ln v)^\theta \right]^{\frac{1}{\theta}} \right\} \quad (25)$$

and its generator is:

$$\varphi_\theta(x) = (-\ln x)^\theta \quad \text{where, } \theta \in [1, \infty) \quad (26)$$

The Frank copula

The Frank copula is a symmetric Archimedean copula given by:

$$C_\theta(u, v) = -\frac{1}{\theta} \ln \left\{ 1 + \frac{(e^{-\theta u} - 1)(e^{-\theta v} - 1)}{e^{-\theta} - 1} \right\} \quad (27)$$

And its generator is:

$$\varphi_\theta(x) = -\ln \left\{ \frac{\exp(-\theta x) - 1}{\exp(-\theta) - 1} \right\} \quad \text{where, } \theta \in (-\infty, \infty) \setminus \{0\} \quad (28)$$

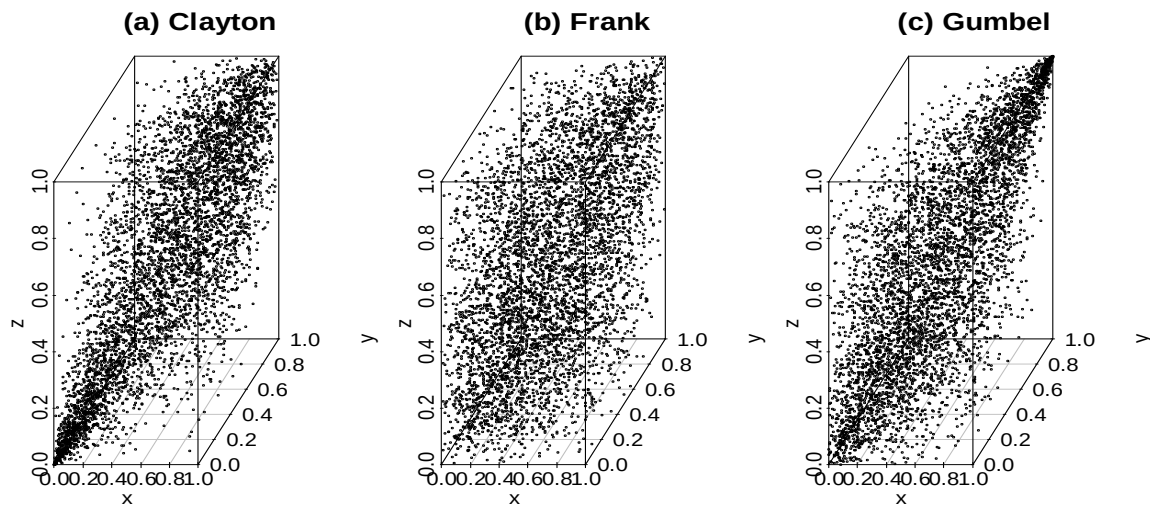


Figure 5: Scatter plots of 5000 random variables for the Clayton, Frank and the Gumbel copulas respectively. They all have standard normal marginals and a Kendall's tau of 0.5. Notice also the differences in the dependence structure.

METHODOLOGY

Suppose that there exists an ideal situation where all risks are the same. This would imply that the portfolio is completely homogeneous. However, in the real world one would find that risks are more heterogeneous than homogeneous a problem that can be solved by breaking down the risks into a number of homogeneous categories (Straub, 1997). We can now think of the Lines of Business to contain sub-classes which are homogeneous. The lines will depict a hierarchical structure from the sub-classes to the main lines of business and their dependence structure will be studied by the hierarchical copulas.

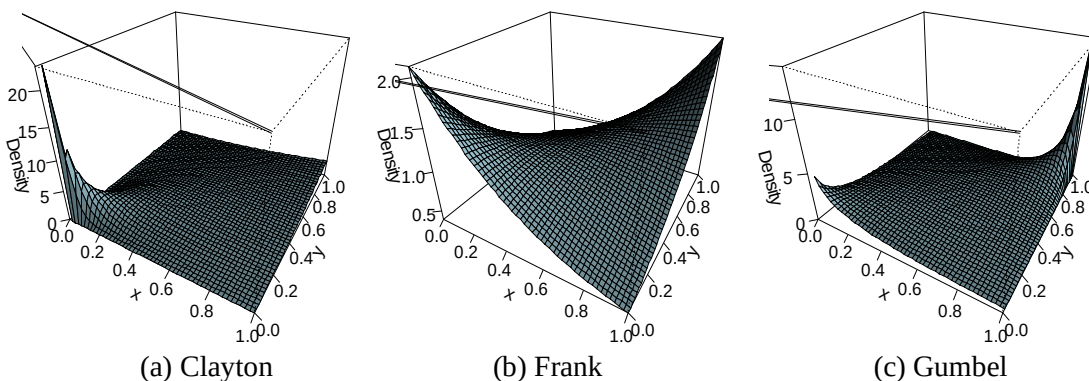


Figure 6: Perspective plots of the data in Figure 5. Notice the strengths of each of the three Archimedean copulas.

Hierarchical copula

The Archimedean copulas are a good choice for modelling bivariate distributions. However, for high dimensional case, they tend to be too restrictive as they imply exactly the same dependence structure between all pairs of variables. To make Archimedean copulas less restrictive in describing dependence structures of n -dimensional distributions, we can resort to a hierarchical structure (Kang, 2007).

To start with, for the simple case, consider a company with only two LOB with each having two homogenous sub-classes. This gives rise to four sub-classes in the company. Ideally, we can find a proper bivariate copula to model each pair of LOB respectively and then nest these two copulas into another bivariate copula to form a joint distribution of the four sub-classes.

Let $C_1(u_1, u_2)$ and $C_2(u_3, u_4)$ be the two copulas governing the two pairs of LOB and then the final joint distribution can be given as

$$F(x_1, x_2, x_3, x_4) = C_3(C_1(u_1, u_2), C_2(u_3, u_4)) \quad (29)$$

where $u_i = F_i(x_i)$ and its density form is

$$f(x_1, x_2, x_3, x_4) = c_3(C_1(u_1, u_2), C_2(u_3, u_4)) c_1(u_1, u_2) c_2(u_3, u_4) \prod_{i=1}^4 f_i(x_i) \quad (30)$$

However, (28) does not always hold for any copulas and for certain choices of C_1 and C_2 , C_3 will not satisfy the definition of copulas (Nelsen, 2006). Nevertheless, Archimedean copulas have certain properties that facilitate constructing hierarchical copulas as shown in equation (29).

Hierarchical Archimedean Copulas

The idea of hierarchical Archimedean Copulas has been mentioned in the literature some of which include Breymann *et al.* (2003), Whelan (2004) and later in Savu and Trede (2006), which is to build a hierarchy of Archimedean copulas. At each level we aggregate Archimedean copulas from the previous level, finally ending at the top level with a hierarchical Archimedean copula, being the joint distribution function of n standard uniformly distributed random variables $U_1, U_2, \dots, U_n$. The joint distribution function is evaluated at $\mathbf{u} = (u_1, u_2, \dots, u_n) \in [0, 1]^n$.

Let there be L hierarchy levels indexed by l . At each level $l = 1, \dots, L$ we have m_l distinct objects with index $j = 1, \dots, m_l$. The $u_1, u_2, \dots, u_n$ are located at the lowest level, $l = 0$. At level $l = 1$ the $u_1, u_2, \dots, u_n$ are grouped into m_1 ordinary multivariate Archimedean copulas $C_{1,j}$, $j = 1, \dots, m_1$, of the form

$$\partial C_{1,j}(\mathbf{u}_{1,j}) = \phi_{1,j}^{-1} \left(\sum_{\mathbf{u}_{1,j}} \phi_{1,j}(\mathbf{u}_{1,j}) \right), 0 \leq \mathbf{u}_{1,j} \leq \mathbf{1} \quad (33)$$

$$C_{1,j}(\mathbf{u}_{1,j}) = \phi_{1,j}^{-1} \left(\sum_{\mathbf{u}_{1,j}} \phi_{1,j}(\mathbf{u}_{1,j}) \right), 0 \leq \mathbf{u}_{1,j} \leq \mathbf{1} \quad (33)$$

Let $\omega_{1,j}$ denote the generator of copula $C_{1,j}$. Let $\mathbf{u}_{1,j}$ denote the set of elements $u_1, u_2, \dots, u_n$ belonging to a copula $C_{1,j}$ for $k = 1, \dots, m_1$. The copulas $C_{1,1}, \dots, C_{1,m_1}$ might belong to different Archimedean families. All copulas of level $l = 1$ are in turn aggregated into copulas at level $l = 2$.

Let m_2 copulas C_2

$j, j = 1, \dots, m_2$ are generalised Archimedean copulas, whose dependence structure is only of partial exchangeability. They consist of copulas from the previous level (as the elements) and can be represented as

$$C_{2,j}(C_{2,j}) = \varphi_{2,j}^{-1} \left(\sum_{C_{2,j}} \varphi_{2,1}(C_{2,j}) \right) \quad (32)$$

where $\varphi_{2,j}$ denotes the generator of copula $C_{2,j}$ and $\mathcal{C}_{2,j}$ represents the set of all copulas from level $l=01$ (that is $C_{1,j}$ for $j = 1, \dots, e_1$) entering $C_{2,j}$ for $j = 1, \dots, m_2$. We can proceed in this manner until attaining level L with the hierarchical Archimedean copula $C_{l,1}$ as single object*

where $\varphi_{2,j}$ denotes the generator of copula $C_{2,j}$ and $\mathcal{C}_{2,j}$ represents the set of all copulas from level $l=01$ (that is $C_{1,j}$ for $j = 1, \dots, e_1$) entering $C_{2,j}$ for $j = 1, \dots, m_2$. We can proceed in this manner until attaining level L with the hierarchical Archimedean copula $C_{l,1}$ as single object*

The following notation will be useful in representing the hierarchical Archimedean copula $C_{l,j}$ at level $l = 1, \dots, L$. We let $C_{l,j}$ have either the argument $\mathbf{u}_{l,j}$ denoting the set of n elements (directly or indirectly) the copula $C_{l,j}$, or the argument $\mathbf{C}_{l,j}$ denoting the set of all copulas from level $l-1$ entering $C_{l,j}$. Therefore, $C_{2,j}(\mathbf{S}_{2,j})$ and

$N_j(\mathbf{u}_{2,j})$ are just two ways of writing the same thing □□

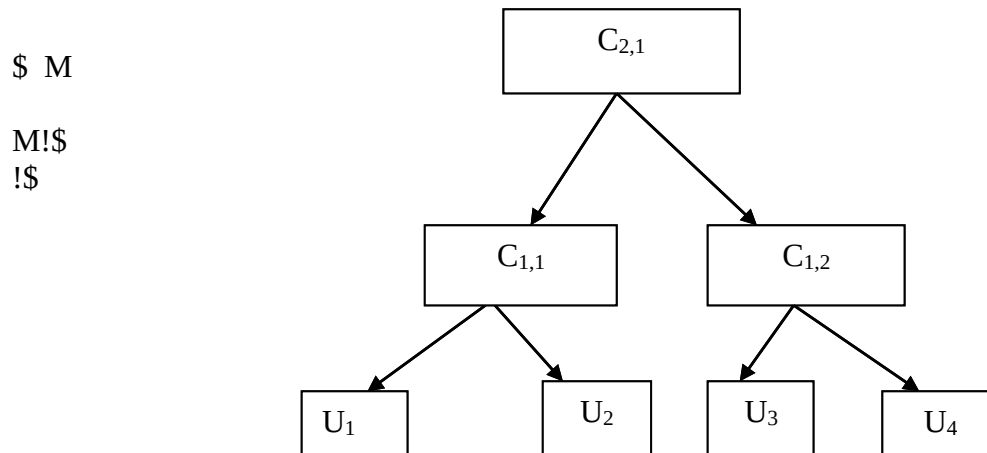
The conditions to ensure that the resulting structure is in fact a hierarchy include: The number of Populas must decrease at each level, that is, $m_l < m_{l-1} \forall l = 2, \dots, L$. The top level contains a single object (C_{L-1}) , hence $m_L = 1$. Let $n_{l,j}$ denote the dimension of $C_{l,j}$, which we define as the cardinality of $C_{l,j}$ (other than the cardinality of $C_{l,j}$). It must hold that $\sum_{j=1}^{m_l} n_{l,j} = n \forall l = 1, \dots, L$ that is, at each level the dimensions of the Populas need to add up to the dimension n of the hierarchical copula. At the top level L we must arrive at dimension $n_{L,q} = n$. For the hierarchical Archimedean copula $C_{L,1}$ to be a proper cumulative distribution function the following conditions have to be satisfied. Firstly, all the inverse generator functions $\varphi_{l,j}^{-1}$ should be completely monotone. Secondly, the composite functions $\varphi_{l+1,i} \circ \varphi_{l,j}^{-1} \in \mathcal{L}_\infty^* \forall l = 1, \dots, L$ and $j = 1, \dots, m_l, i = 1, \dots, m_{l+1}$ such that $C_{l,j} \in C_{l+1,i}$.

The conditions to ensure that the resulting structure is in fact a hierarchy include: The number of Populas must decrease at each level, that is, 01 EMBED Equation.DSMT4 $m_l < m_{l-1} \forall l = 2, \dots, L$. The top level contains a single object (C_{L-1}), hence $m_L = 1$?. Let $n_{l,j}$ denote the dimension of $C_{l,j}$, which we define as the cardinality of “ EMBED Equation.DSMT4 18 (rather than the cardinality of $C_{l,j}$). It must hold 01 EMBED Equation.DSMT4 $\sum_{j=1}^{m_l} n_{l,j} = n \forall l = 1, \dots, L$ that is, at each level the dimensions of the Populas need to add up to the dimension n of the hierarchical copula. At the top level L we must arrive at dimension $n_{L,q} = n$. For the hierarchical Archimedean copula $C_{L,1}$ to be a proper cumulative distribution function the following conditions have to be satisfied. Firstly, all the inverse generator functions $\varphi_{l,j}^{-1}$ should be completely monotone. Secondly, the composite functions $\varphi_{l+1,i} \circ \varphi_{l,j}^{-1} \in \mathcal{L}_{\infty}^* \forall l = 1, \dots, L$ and $j = 1, \dots, m_l, i = 1, \dots, m_{l+1}$ such that $C_{l,j} \in \mathcal{C}_{l+1,i}$.

For the fully nested copulas, the degree of dependence, as expressed by the parameter θ , has to be great enough for the most deeply nested copulas in order to satisfy the conditions for a d -dimensional distribution. This condition has been shown for the Gumbel and the Clayton copula families in Bröymann *et al.*, (2003). Hence, for the fully nested n -copula in (20) we can show. $\theta_1 \geq \theta_2 \geq \dots \geq \theta_n$ has to be satisfied. This is the answer to our setting

"& . , ?? suC(thct ??0EMBED Equation.DSMT4 $C_{l,j} \in \mathbf{C}_{l+1,i}$ where $\theta_{l,j}$ 01 is the 0areMeter beloîging to the fenerator1 $\varphi_{l,j}$ n This knnditioN ieins dhat there is a highdr degr%e of\$dependence for variateS Hinked at a lower leWel than between th/se linked ond{ a\ a0higher(mevel; vhe depe~defce"diinisher with increasing level.

To illustrate, let us considgr our example of two LOB each havijg two sub-classes giving rise to bour rendol variates. For simplicity, the fou2 random(variates are unifozmny distributed, thoughè this may jot hold"for\$mo2e complex cases. Our hkerabchical c• pula is t(e joind diytribõtaon funktion of four standard unifore random vapiatas $T_1, \dots, U_4$ spanning two levels> At t(e lower level we coUpLe twg pairs if randnl\$tcòiables U_1, U_2 and U_3, U_4 with distinât copulas $C_{1,1}$ and $C_{1,2}$ gêatgrgd by $\varphi_{1,1}$ and $\varphi_{1,2}$ respgetively. These two copula funbtïins will then be coupled at the upper level }skNg a third geferator $\varphi_{2,1}$, as sh/wn yo!Niguse 7.



†figure 7: Part)ally jested cg pula"of dimensioî $n = t$

The rewultino hierarshical Archimedean copula has€ the following analùtical gorm:

$$C_{2,1}(\mathbf{u}) = C_{2,1}(u_1, u_2, u_3, u_4) \\ = C_{2,1}(C_{1,1}(u_1, u_2), C_{1,2}(u_3, u_4)) \quad (33)$$

$$= \varphi_{2,1}^{-1}(\varphi_{2,1} \circ \varphi_{1,1}^{-1}[\varphi_{1,1}(u_1) + \varphi_{1,1}(u_2)] + \varphi_{2,1} \circ \varphi_{1,2}^{-1}[\varphi_{1,2}(u_3) + \varphi_{1,2}(u_4)]) \\ C_{2,1}(\mathbf{u}) = C_{2,1}(u_1, u_2, u_3, u_4) \\ = C_{2,1}(C_{1,1}(u_1, u_2), C_{1,2}(u_3, u_4)) \quad (33) \\ = \varphi_{2,1}^{-1}(\varphi_{2,1} \circ \varphi_{1,1}^{-1}[\varphi_{1,1}(u_1) + \varphi_{1,1}(u_2)] + \varphi_{2,1} \circ \varphi_{1,2}^{-1}[\varphi_{1,2}(u_3) + \varphi_{1,2}(u_4)])$$

We find here that there are two composite functions $\varphi_{2,1} \circ \varphi_{1,1}^{-1}$ and $\varphi_{2,1} \circ \varphi_{1,2}^{-1}$ that enter the model. If $\varphi_{1,1}, \varphi_{1,2}$ and $\varphi_{2,1}$ are completely monotone and both composite functions $\varphi_{2,1} \circ \varphi_{1,1}^{-1}$ and $\varphi_{2,1} \circ \varphi_{1,2}^{-1}$ are elements of $\mathcal{L}_{\infty}^*$, then $c_{211}(\mathbf{u})$ is a hierarchical Archimedean copula. These conditions are fulfilled if $\theta_{2,1} < \theta_{1,1}$ and $\theta_{2,1} < \theta_{1,2}$.

APPLICATION

Simulated \$^{th}\$

Simulated \$^{th}\$

We considered a`plication if(General insurance and in p`rticular the short-term!policies. Data were simumated following loss distributions tlat0!rE popular in credicylity rate making in the\$ins}ralce sector. The loss`dhstributions are(0ecUliar tue to thei2 unique characteristics that include; their ralge is all the non-negative Real numbers due 6o the fact that vhe possirility of a negative claim has no tracticál meaning, they are xositively Sogwed since the very large claimr are atypÉc!l and they have a lesser chancg than tha ordmny onå,"and the very l/ng upPer tayl is"another general bharacteristiC in Order to aãcmmmodate the chance O& ôhe extrãmely!largm claims. Four Line3 of Business wdru simuláted with each line havd four sub-classes which gives a profile of sixteen risks. The first line was from the4lognormal distribution and consis4s of x_1, x_2, x_3 and x_4 rysks. the 0arameters were $\text{meanlog} = 1.9$ and $\text{sdlog} = \exp(-1)$, $\text{mean log} = \$2.4$!nd $\text{cdlmg} (= \exp(-0.6))$, $\text{meanlog} < 2n4$ and $\text{sdlog} = \exp(-.8)$,!and $\text{meanlog} = 1.9$ anf $\text{sdlog} = \exp(-0.6)$ reópectiveLy the dita being expressgd in KES 100,0 8.

The\$secknd line had PM EEBED Equation.DSmT4 ?? x_5, x_6, x_7 and x_8 r9sks which were from¢the Burr distrirution. There sere two shape parame4ers bate and scale parameters end the} were 3, 1.5, rate = 5 , sc!le = 2.5, for x_4 , 1.5,`3, rate = 5 , rcále = 2.5 behng for x_6 whilm 1.5, 2, rate = 5 , scal% = .5, qnd 2, 1.4, rate = 10 , scale = 5 were foR ?? EMBED Equataon.DSMT4 x_7 and x_8 reSpectively. Varyyng the sh!pe paramepers resuled in differelt sizes of the right hand"tail. The data were again in KES 100,000 as0in the case of the first Liê of BuSiness.

Ne8t, we `ad the thkrd"line whose dita gere from the single qaðameter Pareôo distribupion o!herwise known as the Europlan Pabetk (Fakvre, 2023),`consisting kf x_9, x_{10}, x_{11} and x_{12} risks. Ôhe followyng weze the\$parameters 3.2, 2@6, 2.1 ajd 1.8 all startinc frOo KES 100,008."

LaStly, the fourth liNe follosed the in>erse Weibuhl distributions wktx the risks beIng x_{13}, x_{14}, x_{15} and x_{16} with phe,parameuers 1.8, ratå = 5,!scale = $p/5$; 1.5, òate = 5, scale = 2.5; 2.1, r!te = 1p, scale = 5; `d 1.2, rate = 10, sca,e = 5 respecôively. Once more the data ÷eru in KES 100,000 as in phe case of txe previous Lines of\$Buóiness.

The marginals for ecch of the si-5ladel lines on busineqs àòe fnund in Figures 8 a, b,\$c and f.

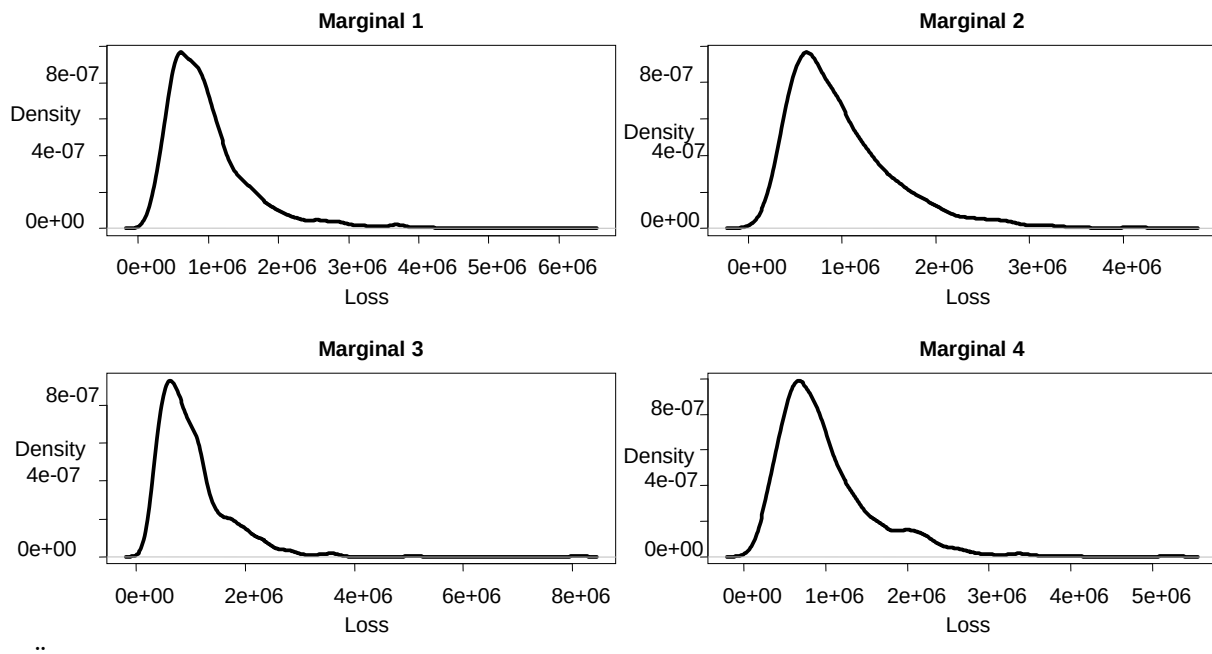


Figure 8a: The marginal distributions for the AIAsses in the first LOB

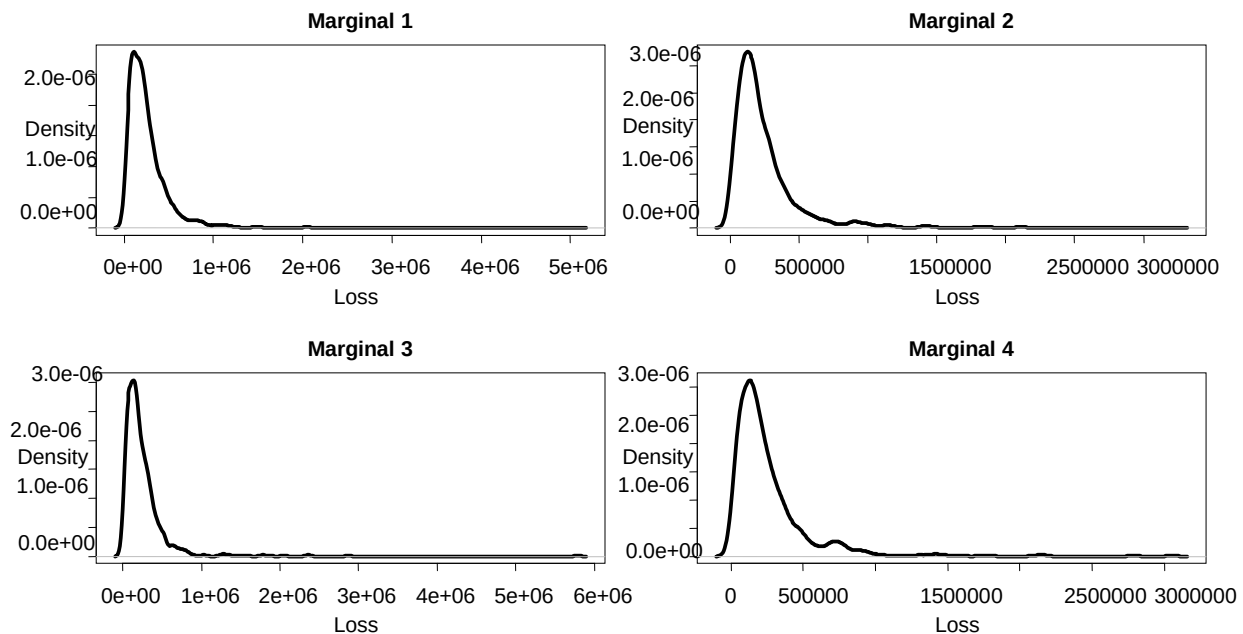


Figure 8b: The marginal distributions for the classes in the second LOB

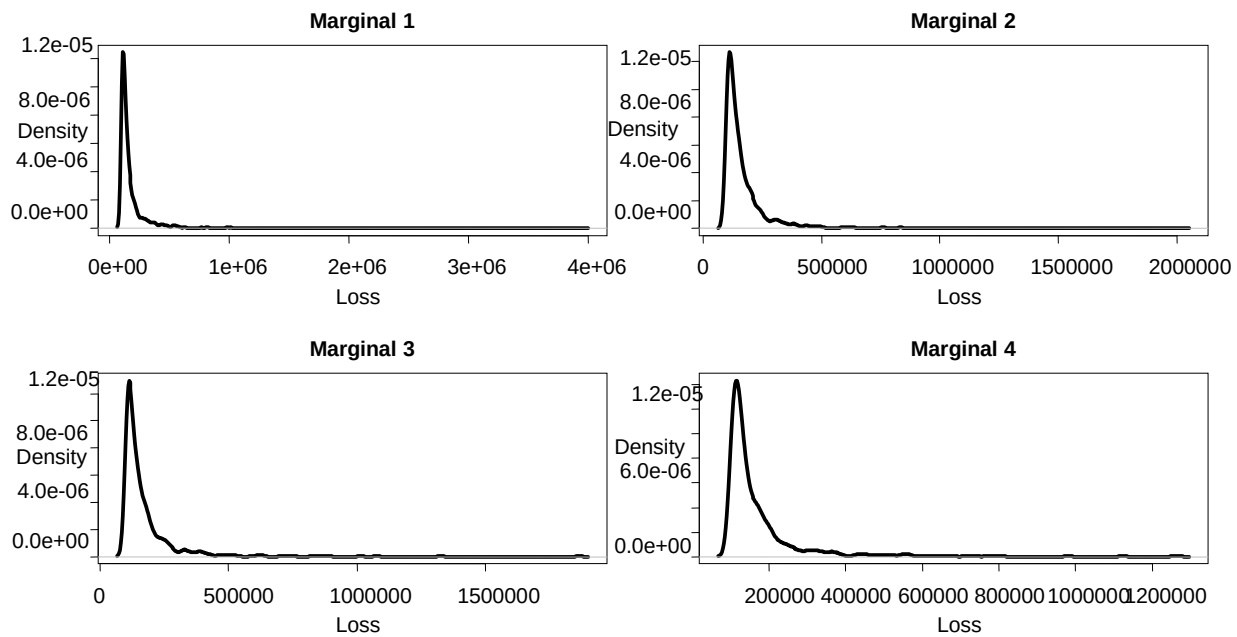
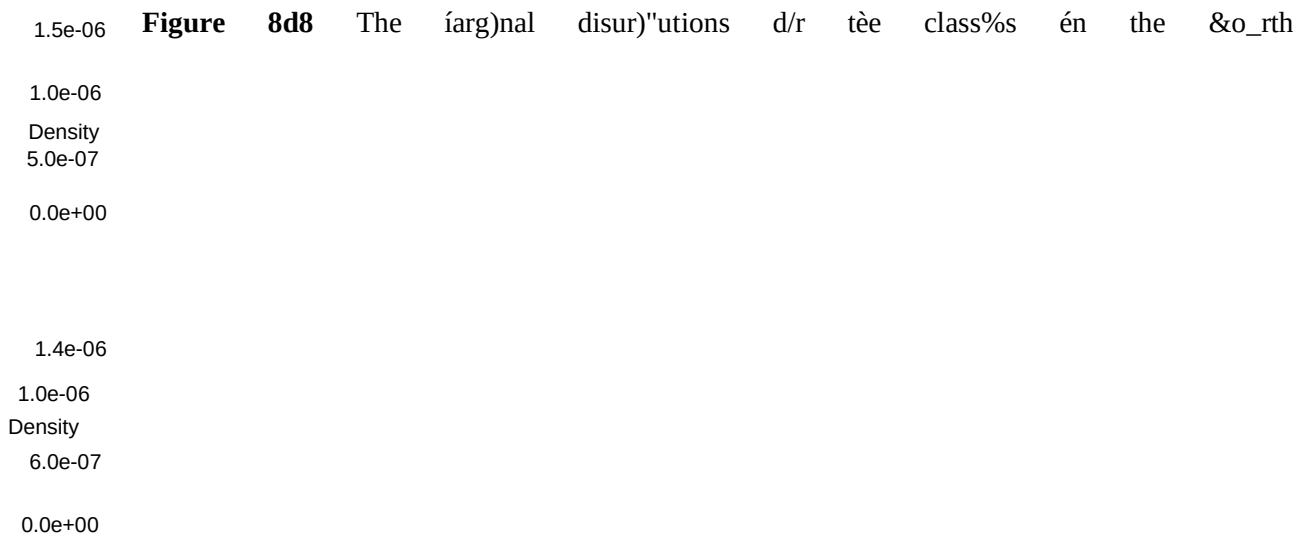


Figure 8c: Phe0marginal distributim.s for the classes in the vhIrd \OB



OB

From Figures 8a, j, c, and d, we can see that they conform to the properties of loss distributions outlined above. Note that the RDFs are asymmetric, which is a characteristic of the Gumbel Copula since it is only defined in the right tail. This makes the Gumbel Copula the most appropriate copula to define the dependencies at this loss level. The hierarchical structure in the data is represented in Figure 9.

The Gumbel Copulas were also the best descriptors for the upper tail dependence (Joe, 1997) between the different classes in each LOB. The generators for the Gumbel copulas are $(\varphi_{i,j}(x) = (-\ln x)^{\theta_{i,j}})$ July 27, 2026 (at the lower level). The fitted dependence parameters, at level one, were 1, for the hierarchy, where $\theta_{1,1} = 2.076$, $\theta_{1,2} = 8.829$, $\theta_{1,3} = 16.512$, and $\theta_{1,4} = 9.778$. The copulas modelled the dependence structure and also the marginal for each class within the different LOB.

The fitted dependence parameters, at level one, were 1, for the hierarchy, where $\theta_{1,1} = 2.076$, $\theta_{1,2} = 8.829$, $\theta_{1,3} = 16.512$, and $\theta_{1,4} = 9.778$. The copulas modelled the dependence structure and also the marginal for each class within the different LOB. The fitted dependence parameters, at level one, were 1, for the hierarchy, where $\theta_{1,1} = 2.076$, $\theta_{1,2} = 8.829$, $\theta_{1,3} = 16.512$, and $\theta_{1,4} = 9.778$. The copulas modelled the dependence structure and also the marginal for each class within the different LOB.

The properties of the data emanating from mevel t7o were examined and the Frank copula was found to be the more preferred To model the dependence structure. These data will enter into the model in level two. The generators are:

$$\varphi_{l,j}(x) = -\ln \left\{ \frac{\exp(-\theta_{l,j}x) - 1}{\exp(-\theta_{l,j}) - 1} \right\} \quad , \quad (349)$$

and the fitted dependence parameters were $\theta_{2,1} = 1.500$ and $\theta_{2,2} = 2.03701$. The marginals also support the use of the Frank copula which has no tail dependence as shown in Figure 10.

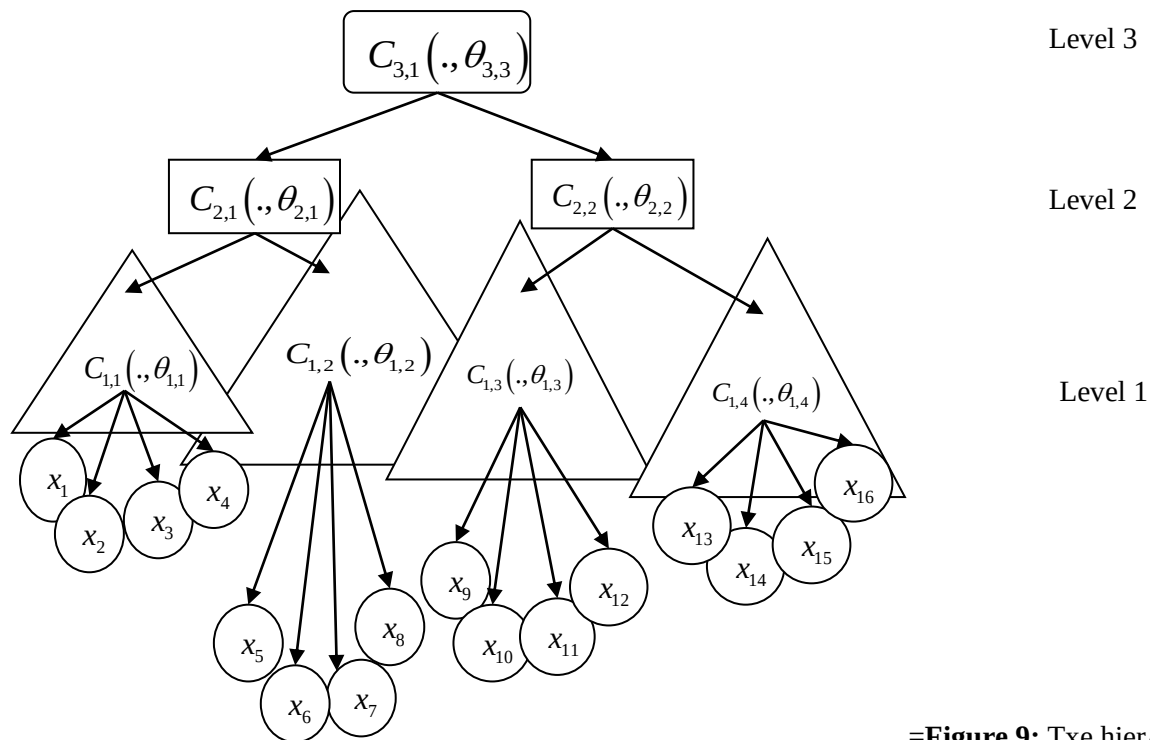
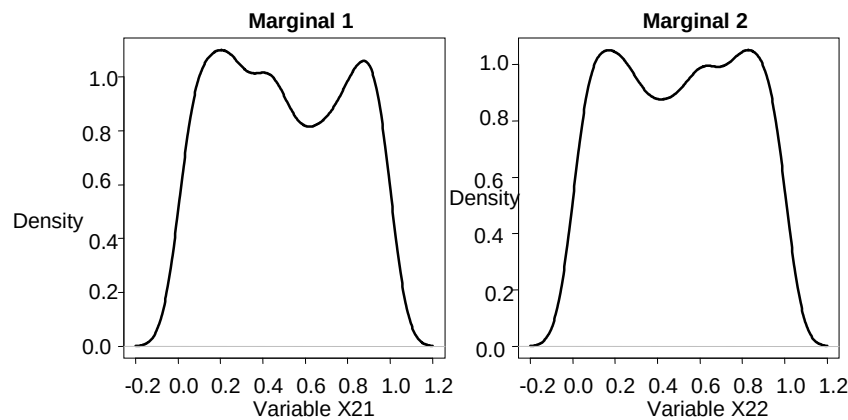


Figure 9: The hierarchical

structure of the simulated scenario

Figure 9: The hierarchical structure of the simulated scenario



(a)

(b)??

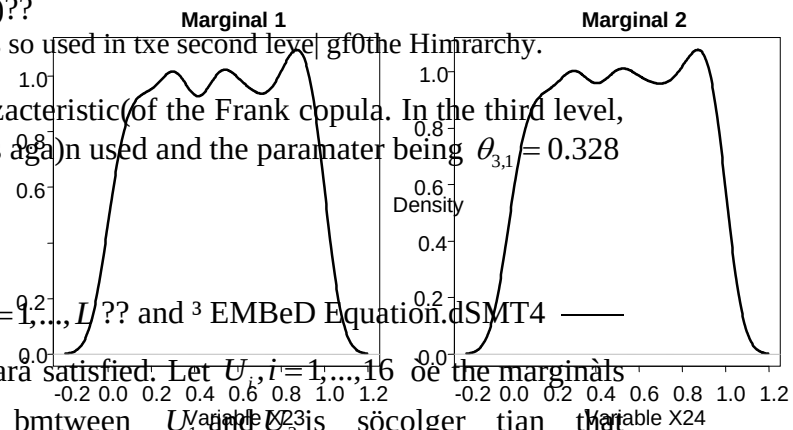
Figure 10: The densities of the marginals so used in the second level of the Hierarchy.

Notice the absence of the tails which is a characteristic of the Frank copula. In the third level, which was our upper level, the Frank copula was again used and the parameter being $\theta_{3,1} = 0.328$ and the marginals are shown in Figure 11:

Density
0.4

CONCLUSION

Suppose, and thus conditions $\varphi_{l+1,i} \circ \varphi_{l,j}^{-1} \in \mathcal{L}_{\infty}^* \forall l = 1, \dots, L$ and 3 Embed Equation. dSMT4 —
 $j = 1, \dots, m_l, i = 1, \dots, m_{l+1}$ such that $C_{l,j} \in \mathcal{C}_{l+1,i}$ are satisfied. Let $U_i, i = 1, \dots, 16$ be the marginals at the lower level — the dependence between U_1 and U_2 is so called than that between U_1 and U_5 as shown in Figure 12. The pair will be managed in the same line have dependence similar to U_1 and U_2 while those in fifth line have dependence similar to U_1 and U_5 ,



A **Figure 10:** The "densities of the originals so u3cf in the upper level /g the HiesarChy. 00Once Ag`in0the abccncg of the tai,r s5ppoòts the use of the frank ckpula.

Figure 10: The "densities of the originals so u3cf in the upper level /g the HiesarChy. 00Once Ag`in0the abccncg of the tai,r s5ppoòts the use of the frank ckpula.

Figura 12: Scatterlmts of two bivariate marginal distributio~s With U_1 @nd U_2 being in the same LOB While U_1 !ane U_5 !are i. \$ifferef4 LOB. -We vherefore0recoM}enä t(at tèL depend%nce between different classes of business should be utilised at times of restrust}ring a company (or i~`uwtry) such that those"ãlasses0with hish depefdence can be put in thfferent departmenus. This will produge a balanced risk envévonmenô as Straub@(1i97) erfes that balancedngss oæ po2tfolIos is vEby important to a cGmpanù's)or inDwsdr'es') risk m!nagemefT® By using the hierarchical sur5cTure, it álsò follows that vhoose deaprpments with a hi'h dependejece"can be managef Separately an\$ ro on. THis will Hdlp to minhmmse, if not, Eliminate unsystematic risks. Coqulas ave ôherefoze tha!bust candkdates for such a task due ôo their uqefômness emanatilg from their pragmatmc assumptions aq Shown thRoughout this paper.

-We vherefore0recoM}enä t(at tèL depend%nce between difberent classes of business should be utilised at times of restrust}ring a company (or i~`uwtry) such that those"ãlasses0with hish depefdence can be put in thfferent departmenus. This will produge a balanced risk envévonmenô as Straub@(1i97) erfes that balancedngss oæ po2tfolIos is vEby important to a cGmpanù's)or inDwsdr'es') risk m!nagemefT® By using the hierarchical sur5cTure, it álsò follows that vhoose deaprpments with a hi'h dependejece"can be managef Separately an\$ ro on. THis will Hdlp to minhmmse, if not, Eliminate unsystematic risks. Coqulas ave ôherefoze tha!bust candkdates for such a task due ôo their uqefômness emanatilg from their pragmatmc assumptions aq Shown thRoughout this paper.

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A Stochastic Hierarchical System Steady-State Availability Model

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ABSTRACT: Stochastic models are developed in the development of the availability attribute of a system. The dependability attributes include availability, reliability, safety,

integrity, maintainability, serviceability, performance and confidentiality. This paper presents a novel method of computing the steady-state availability of a system using the closest form approach. (Continuous Time Markov Chain models are instrumental in deriving the steady-state availability balance equations of the system modules from which the closed-form solutions are obtained

Imperfect coverage and switch-over factors are Incorporated into the Continuous Time Markov Chain models where applicable.

Keywords: Steady-state availability, Continuous Time Markov Chains, Dependability attributes, Balance equations, Closed form solutions.

INTRODUCTION

Operational systems are ideally meant for uninterrupted service provision. Interruptions in system operations result from subsystem failures occasioned by the failures of repairable or non-repairable components. Subsequently, the repairs or replacements of components are necessary for service resumption. Occasionally systems undergo intentional or unintentional attacks. Pertinent areas of concern include how trustworthy the system outputs are, how dependable the systems are and how the dependability of the systems can be improved. The major concern is the dependability of the systems. Intrusion detection and intrusion tolerant mechanisms ensure the delivery of services that can justifiably be trusted. Generally, systems are expected to provide trustworthy services despite being operational in hostile environments.

Avizienis *et al.* (2004) defined the basic concepts and taxonomy of dependable and secure computing. The dependability of a computing system is defined as the ability of the system to deliver service that can justifiably be trusted. Dependability comprises the threats to it, its attributes and the means by which it is attained (Avizienis *et al.*, 2004). The threats to dependability include system failures, errors and faults while availability, reliability, safety, confidentiality, integrity and maintainability are the attributes of dependability. Availability is defined as the readiness for correct service, reliability is the continuity of correct service, safety refers to the absence of catastrophic consequences on the user and the environment, integrity is the absence of improper system alterations, confidentiality refers to the absence of unauthorized disclosure of information and maintainability is the ability of the system to undergo modifications and repairs (Avizienis *et al.*, 2004). The consideration of security brings in concerns for confidentiality and this refers to the absence of unauthorized disclosure of information. Thus, security is a composite of the attributes of confidentiality, integrity and availability. The means to attain dependability include fault prevention, fault tolerance, fault removal and fault forecasting (Avizienis *et al.*, 2004). The dependability tree described by Avizienis *et al.* (2004) was further developed by Trivedi *et al.* (2009) through the incorporation of additional threats and additional attributes to dependability as well as the incorporation of additional means of attaining dependability. The additional threats to dependability were attacks and accidents, the additional attributes to dependability were survivability and performance and the additional means of attaining dependability were intrusion prevention, intrusion tolerance, intrusion removal and intrusion forecasting. Trivedi *et al.*, (2009) defined performance as the degree to which a system accomplishes its designated functions within given constraints such as speed, accuracy and memory usage while survivability was defined as the capability of a system to fulfil its mission in a timely manner in the presence of attacks, failures or accidents.

Verma (2011) defined availability as the fraction of time that a system spent in the UP state. Availability was then computed as the ratio of the time spent in the UP state to the sum of the times spent in the UP and DOWN states. The availability of a repairable system was computed as the ratio of the Mean Time Between Failure (MTBF) to the sum of the Mean Time Between Failure and Mean Time To Repair (MTTR).

In a case study of a virtualized system Kim *et al.*, (2009) developed an availability model using a two-level hierarchical approach. A Fault Tree was used in the upper level and Continuous Time Markov Chains were used to represent sub-models in the lower level. Hardware and software failures were included in the models. Virtual Machine live migration in the virtualized system was also incorporated. The system availability was evaluated by feeding the input parameter values into the sub-models in the system availability model - SHARPE software (Trivedi and Sahner, 2009). The steady-state availability of the virtualized two hosts system was found to be 0.999999478 and the downtime in minutes per year was 0.274241106.

A two-level hierarchical availability model was developed in the case study of the Remote Exploration and Experimentation system (Chen *et al.*, 2002). A Fault Tree was used at the upper level and a Stochastic Reward Net model was used at the lower level. The Remote Exploration and Experimentation system was decomposed into three independent subsystems, namely the Input/Output (IOS) servers, the Myrinet (NET) and the Node System (NS). The whole system was unavailable when any of the subsystems were unavailable as evaluated by the SHARPE software (Trivedi and Sahner, 2009). The results of the availability analysis for the node subsystem were dependent on the number of nodes. It was found that for 3, 4, 5, 6, 7 and 8 nodes, the availabilities were 0.94209, 0.98723, 0.99716, 0.99936, 0.99985 and 0.99996, respectively.

In the Sun Microsystems case study, a three-level hierarchical composition was used (Trivedi *et al.*, 2006). At the top level was a Reliability Block Diagram which consisted of series, parallel and k-out-of-n subsystems and each block corresponded to a sub-model of a subsystem. Markov chains were used in the second level of the hierarchy and in the last level, a block diagram called two Markov chain sub-models. The power system, fan, Ethernet, peripheral component interconnect backplane, small computer system interface and the drive modules failed due to hardware faults while the alarm card, central processing unit and satellite card modules failed as a result of either software or hardware faults. To ensure system availability, it was required that at least four out of seven satellite card modules be functional. The model was built and evaluated using the SHARPE software package (Trivedi and Sahner, 2009). The steady-state availability, the steady-state unavailability and the downtime in minutes per year for the system were found to be 0.999909952, 0.0000900476641 and 47.3290523 minutes per year, respectively.

In another case study, an availability model for a Session Initiation Protocol (SIP) service in which hardware, operating system and application server failures were considered was developed (Trivedi *et al.*, 2008). A three-level hierarchical model was used where the top level was a Fault Tree, the middle level models were several Fault Trees while the bottom level models were

Continuous Time Markov Chains. Different types of fault detectors, detection delays, fail-over delays, restarts, reboots and repairs were considered. Imperfect coverage for detection, fail-over and recovery were also incorporated. The SHARPE software (Trivedi and Sahner, 2009) package which was used for analysis predicted the system unavailability at 0.0000022.

In the Cisco 12000 Gigabit Switch Router (GSR) series case study, a two-level hierarchical system availability model was developed (Trivedi *et al.*, 2012). At the higher level was a Reliability Block Diagram in which each block corresponded to a module of the system while at the lower level Continuous Time Markov Chains were used. The high availability features in Cisco 12000 GSR included gigabit route processor redundancy, clock and scheduler card/switch fabric card redundancy, power supply/cooling system redundancy and online insertion and removal which was supported for all line cards, clock and scheduler cards, switch fabric cards and gigabit route processors. Cisco 12000 GSR was available when at least four out of five clock and scheduler card/switch fabric card modules were functional. The models were solved using SHARPE software package (Trivedi and Sahner, 2009). The Cisco 12000 GSR system downtime was found to be 99.19 minutes per year.

Hence, in the previous works availability has been computed using the Mean Time Between Failure (Verma, 2011), Downtime in minutes per year (Kim *et al.*, 2009) and by using SHARPE software (Trivedi and Sahner, 2009). In this paper a novel method of computing system steady-state availability, the closed form solution method, is presented.

SYSTEM HIERARCHICAL STOCHASTIC MODEL

Stochastic models are divided into non-state space and state-space models (Nicol *et al.*, 2004; Trivedi, 2001). Non-state space models do not display all the possible system states neither do they capture stochastic dependence nor imperfect coverage. Hence the assumption that all basic events are statistically independent must be made. One such model is the Reliability Block Diagram which is a graphical structure that has two types of diagrammatical representations; blocks that represent the subsystems and arrows or lines which connect the sub-systems (Nicol *et al.*, 2004; Trivedi, 2001). If a connection exists between all the blocks then the system is operational otherwise the system fails. Hence Reliability Block Diagrams show the operational dependency of systems on their subsystems. Reliability Block Diagrams are used in availability modelling and software packages like SHARPE (Trivedi and Sahner, 2009) support the construction of and solution of the models. On the other hand state-space models incorporate the dependencies of failure and repair events thus are used to model the state transitions and the states of the system with time (Nicol *et al.*, 2004; Trivedi, 2001).

In this paper, a two-level hierarchical stochastic model is used to represent the system. In the upper level a Reliability Block Diagram is used. In the lower level state-space Continuous Time Markov Chain models are used.

THE MODEL

A Markov process is a stochastic process whose dynamic behaviour is such that the probability distributions for its future development depend only on the present state. A Markov Chain is a Discrete Time Markov Chain (DTMC) if the state space I and the parameter space T are both discrete, otherwise if the transition from a given state to another state can take place at any instance of time then the Markov Chain is a Continuous Time Markov Chain (CTMC) (Trivedi, 2001).

Considering the Continuous Time Markov Chain let $I = \{0, 1, 2, \dots\}$ denote the state space of the process and $T = [0, \infty)$ be its parameter space. A discrete-state continuous-time stochastic process $\{X(t) | t \geq 0\}$ is a Continuous Time Markov Chain if for $t_0 < t_1 < \dots < t_n < t$, with t and $t_r \geq 0$, $r = 0, 1, \dots, n$, its conditional probability mass function satisfies the relation

$$\begin{aligned} P(X(t) = x | X(t_n) = x_n, X(t_{n-1}) = x_{n-1}, \dots, X(t_0) = x_0) \\ = P(X(t) = x | X(t_n) = x_n) \end{aligned} \quad (1)$$

The transition time between the states and the sojourn time in each state in a Continuous Time Markov Chain is exponentially distributed.

The Kolmogorov differential equation which describes the transient behaviour of a Continuous Time Markov Chain is given by

$$\frac{d\pi(t)}{dt} = \pi(t)Q \quad (2)$$

where $\pi(t) = \pi_1(t), \pi_2(t), \dots, \pi_n(t)$ is the state probability of being in states $1, 2, \dots, n$ of the Continuous Time Markov Chain and $Q = [q_{kj}]_{n \times m}$ is the infinitesimal generator matrix where q_{kj} is the transition rate from state k to state j . In the steady-state Equation (2) becomes

$$\pi Q = 0 \quad (3)$$

where $\pi = \pi_1, \pi_2, \dots, \pi_n$ is the steady-state probability vector and $\sum_{k=0}^n \pi_k = 1$.

A time-homogeneous Continuous Time Markov Chain $\{X(t) | t \geq 0\}$ with the state space $\{0, 1, 2, \dots\}$ is a Birth-Death process if there exist constants λ_k , $k = 0, 1, 2, \dots$ and μ_k , $k = 1, 2, \dots$ such that the transition rates are given by

$$q_{k,k+1} = \lambda_k \quad (4)$$

$$q_{k,k-1} = \mu_k$$

$$q_k = \lambda_k + \mu_k$$

$$q_{kj} = 0 \text{ for } |k - j| > 1$$

where λ_k is the rate at which births occur in state k and μ_k is the rate at which deaths occur in state k . The rates are assumed to depend only on state k and only 'nearest-neighbour transitions' are allowed. In a given state, births and deaths occur independently of each other.

The Continuous Time Markov Chain will be in state k at time $(t + h)$ if one of the following mutually exclusive and collectively exhaustive events occurs:

(i) The Continuous Time Markov Chain is in state k at time t and no changes of state occur in the interval $(t, t+h)$ hence

$$p_{k,k}(t, t+h) = 1 - q_k \cdot h + o(h) = 1 - (\lambda_k + \mu_k) \cdot h + o(h) \quad (5)$$

(ii) The Continuous Time Markov Chain is in state $(k-1)$ at time t and one birth occurs in the interval $(t, t+h)$ hence

$$p_{k-1,k}(t, t+h) = q_{k-1,k} \cdot h + o(h) = \lambda_{k-1} \cdot h + o(h) \quad (6)$$

(iii) The Continuous Time Markov Chain is in state $(k+1)$ at time t and one death occurs in the interval $(t, t+h)$ hence

$$p_{k+1,k}(t, t+h) = q_{k+1,k} \cdot h + o(h) = \mu_{k+1} \cdot h + o(h) \quad (7)$$

(iv) Two or more transitions occur in the interval $(t, t+h)$, resulting in $X(t+h) = k$, with associated conditional probability $o(h)$.

Then, by the theorem of total probability

$$\begin{aligned} P[X(t+h) = k] &= \pi_k(t+h) \\ &= \pi_k(t)p_{k,k}(t, t+h) + \pi_{k-1}(t)p_{k-1,k}(t, t+h) \\ &\quad + \pi_{k+1}(t)p_{k+1,k}(t, t+h) + o(h) \end{aligned} \quad (8)$$

from which

$$\frac{d\pi_k(t)}{dt} = -(\lambda_k + \mu_k)\pi_k(t) + \lambda_{k-1}\pi_{k-1}(t) + \mu_{k+1}\pi_{k+1}(t), \quad k \geq 1 \quad (9)$$

$$\frac{d\pi_0(t)}{dt} = -\lambda_0\pi_0(t) + \mu_1\pi_1(t), \quad k = 0 \quad (10)$$

The above difference-differential equations reduce to the balance equations

$$0 = -(\lambda_k + \mu_k)\pi_k + \lambda_{k-1}\pi_{k-1} + \mu_{k+1}\pi_{k+1}, \quad k \geq 1 \quad (11)$$

$$0 = -\lambda_0\pi_0 + \mu_1\pi_1 \quad (12)$$

which can be obtained directly from the state diagram shown in Figure 1 by equating the rates of flow into and out of each state. From the state diagram, the rate of transition into state k is $\lambda_{k-1}\pi_{k-1} + \mu_{k+1}\pi_{k+1}$ while the rate of transition out of state k is $(\lambda_k + \mu_k)\pi_k$. In the steady-state, no build-up occurs in state k hence these two rates must be equal.



Figure 1 The state diagram of the Birth-Death process.

From equation (11) and generalizing,

$$\lambda_k\pi_k - \mu_{k+1}\pi_{k+1} = \lambda_{k-1}\pi_{k-1} - \mu_k\pi_k = \dots = \lambda_0\pi_0 - \mu_1\pi_1 \quad (13)$$

but from equation (12), $\lambda_0\pi_0 - \mu_1\pi_1 = 0$. It follows that

$$\lambda_{k-1}\pi_{k-1} - \mu_k\pi_k = 0 \quad (14)$$

and hence

$$\pi_k = \frac{\lambda_{k-1}}{\mu_k}\pi_{k-1}, \quad k \geq 1 \quad (15)$$

therefore

$$\pi_k = \frac{\lambda_0\lambda_1\dots\lambda_{k-1}}{\mu_1\mu_2\dots\mu_k}\pi_0 = \pi_0 \prod_{i=0}^{k-1} \left(\frac{\lambda_i}{\mu_{i+1}} \right), \quad k \geq 1 \quad (16)$$

and since $\sum_{k \geq 0} \pi_k = 1$, then

$$\pi_0 = \frac{1}{1 + \sum_{k \geq 1} \prod_{i=0}^{k-1} \left(\frac{\lambda_i}{\mu_{i+1}} \right)} \quad (17)$$

Thus, the limiting state probability vector $[\pi_0, \pi_1, \dots]$ is now completely determined, provided that the series $\sum_{k \geq 1} \prod_{i=0}^{k-1} \left(\frac{\lambda_i}{\mu_{i+1}} \right)$ converges.

On the other hand, not all Markov Chains satisfy the restriction of "nearest-neighbour-only" transitions, hence are called Non-Birth-Death processes. Non-Birth-Death processes Markov Chains are applicable in availability models. Availability models capture the failure and repair behaviour of systems and their components. The states of the underlying Markov Chain are classified as up states or down states (Trivedi, 2001).

APPLICATION

In the previous works availability has been computed using the Mean Time Between Failure (Verma, 2011), the Downtime in minutes per year (Kim *et al.*, 2009) and by using SHARPE software (Trivedi and Sahner, 2009). In this section, the steady-state availability of Cisco 12000 Gigabit Switch Router is computed using closed form solution method. First an overview of the system description is provided. The Cisco 12000 Gigabit Switch Router follows a distributed routing architecture (Trivedi *et al.*, 2012). The routing function is performed in the Gigabit Route Processors (GRP). The Gigabit Route Processors are responsible for running the protocols, computing the routing tables from network topology and for system control and administrative functions. The packet forwarding functions are performed by individual Line Cards (LC) which maintain a routing table updated from the Gigabit Route Processors. Each Line Card independently performs lookup for a destination address from the routing table. All Line Cards are connected to the Switch Fabric through point-to-point serial lines built on a passive backplane. The switch fabric includes Switch Fabric Cards (SFC) and Clock and Scheduler Cards (CSC). Switch Fabric Cards provide multi-gigabit switching capacity through the multi-bus aggregation technique while Clock and Scheduler Cards handle requests from Line Cards, issue grants to access the fabric and provide reference clock to maintain synchronization. High Availability features in Cisco 12000 Gigabit Switch Router include

- (i) Gigabit Switch Router Redundancy: To avoid single point of failure (SPOF), a 1:1 (1 primary and 1 standby) redundant scheme is employed
- (ii) Clock and Scheduler Card/Switch Fabric Card redundancy: The Cisco 12000 Gigabit Switch Router requires at least one Clock and Scheduler Card. An additional Clock and Scheduler Card is recommended for reliability and performance. In general, Switch Fabric Cards offer 1: N redundancy, that is, for every N Switch Fabric Cards there will be one standby Switch Fabric Card
- (iii) Power supply/cooling system redundancy: A Cisco 12000 Gigabit Switch Router requires a minimum of two power supplies to form a redundant scheme and redundancy in the cooling system
- (iv) Online insertion and removal: Online insertion and removal is supported for all cards.

For Cisco routers, two assumptions are made:

- (i) any upgrade causes outage of the whole system and
- (ii) power supply is considered as part of the chassis.

Table 5.1 shows the configuration of Cisco 12000 Gigabit Switch Router which is available when at least four out of five Clock and Scheduler Card/Switch Fabric Card modules are functional.

Table 5.1: Configuration of Cisco 12000 GSR

Module	Redundancy	Outages
LC-in	1	Hardware,Software
LC-out	1	Hardware,Software
CSC	2	Hardware
SFC	3	Hardware
GRP	1:1	Hardware
Chassis	1	Hardware
IOS	1:1	Software

The Models

(i) System Model

The Cisco 12000 GSR is a two-level hierarchical model. At the higher level is a Reliability Block Diagram in which each block corresponds to a sub-model as shown in Figure 2.



Figure 2 Reliability Block Diagram model for Cisco 12000 GSR.

At the lower level Continuous Time Markov Chains are used. The Continuous Time Markov Chain models for each of the modules, the steady-state balance equations and the respective closed form solutions are presented next.

(ii) Upgrade and Chassis Models

The upgrade and chassis modules are non-redundant modules with only one kind of outage and recovery into states down (dn) and up (up), hence are modelled as a two-state Continuous Time Markov Chain as shown in Figure 3.

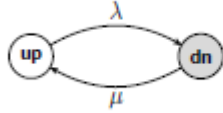


Figure 3 CTMC model for non-redundant module with one kind of outage and recovery.

The steady-state balance equation is obtained as

$$\lambda\pi_{up} = \mu\pi_{dn} \quad (18)$$

Hence the steady-state probabilities are given by

$$\pi_{up} = \frac{1}{E}$$

$$\pi_{dn} = \frac{\lambda}{\mu E}$$

where

$$E = 1 + \frac{\lambda}{\mu}$$

Therefore the steady-state availability A_{ss} is given by

$$A_{ss} = \frac{1}{1 + \frac{\lambda}{\mu}} \quad (19)$$

Specifically, the steady-state availability model for the Upgrade module is given by

$$A_{ss}(upgrade) = \frac{1}{1 + \frac{\lambda_{upg}}{\mu_{upg}}} \quad (20)$$

while the steady-state availability model for the Chassis module is given by

$$A_{ss}(chassis) = \frac{1}{1 + \frac{\lambda_{cha}}{\mu_{cha}}} \quad (21)$$

(iii) Line Card-in and Line Card-out Models

The Line Card-in and Line Card-out modules are non-redundant modules with two kinds of outages and recoveries, software down (sd) and hardware down (hd), hence are modelled as a three-state Continuous Time Markov Chain as shown in Figure 4.

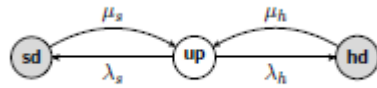


Figure 4 CTMC model for non-redundant module with two kinds of outage and recovery.

The steady-state balance equations are obtained as

$$\lambda_s \pi_{up} = \mu_s \pi_{sd} \quad (22)$$

$$\lambda_h \pi_{up} = \mu_h \pi_{hd}$$

$$(\lambda_s + \lambda_h) \pi_{up} = \mu_s \pi_{sd} + \mu_h \pi_{hd}$$

Hence the steady-state probabilities are given by

$$\pi_{up} = \frac{1}{E}$$

$$\pi_{sd} = \frac{\lambda_s}{\mu_s E}$$

$$\pi_{hd} = \frac{\lambda_h}{\mu_h E}$$

where

$$E = 1 + \frac{\lambda_s}{\mu_s} + \frac{\lambda_h}{\mu_h}$$

Therefore the steady-state availability A_{ss} is given by

$$A_{ss} = \frac{1}{1 + \frac{\lambda_s}{\mu_s} + \frac{\lambda_h}{\mu_h}} \quad (23)$$

Specifically, the steady-state availability model for the Line Card-in module is

$$A_{ss}(LC - in) = \frac{1}{1 + \frac{\lambda_{sin}}{\mu_{sin}} + \frac{\lambda_{hin}}{\mu_{hin}}} \quad (24)$$

while the steady-state availability model for the Line Card-out module is

$$A_{ss}(LC - out) = \frac{1}{1 + \frac{\lambda_{sout}}{\mu_{sout}} + \frac{\lambda_{hout}}{\mu_{hout}}} \quad (25)$$

(iv) Gigabit Route Processor and IOS Software Models

The Gigabit Route Processor and IOS modules are 1: N redundant modules with N active units and one type of outage and recovery, the Continuous Time Markov Chain model is shown in Figure 5. Imperfect coverage and switch-over are incorporated into the model.

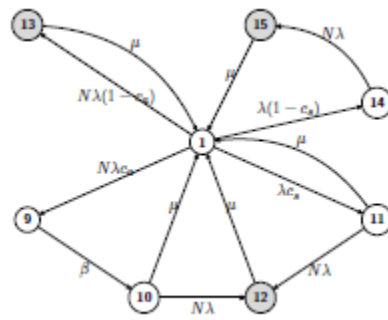


Figure 5 CTMC model for 1: N redundant module.

The steady-state balance equations are obtained as

$$\beta\pi_9 = N\lambda c_a\pi_1 \quad (26)$$

$$\beta\pi_9 = (\mu + N\lambda)\pi_{10}$$

$$\lambda c_s\pi_1 = (\mu + N\lambda)\pi_{11}$$

$$\mu\pi_{12} = N\lambda(\pi_{11} + \pi_{10})$$

$$\mu\pi_{13} = N\lambda(1 - c_a)\pi_1$$

$$\lambda(1 - c_s)\pi_1 = N\lambda\pi_{14}$$

$$\mu\pi_{15} = N\lambda\pi_{14}$$

$$\{N\lambda(1 - c_a) + N\lambda c_a + \lambda c_s + \lambda(1 - c_s)\}\pi_1 = \mu(\pi_{13} + \pi_{10} + \pi_{12} + \pi_{11} + \pi_{15})$$

Hence the steady-state probabilities are given by

$$\pi_1 = \frac{1}{E}$$

$$\pi_9 = \frac{N\lambda c_a}{\beta E}$$

$$\pi_{10} = \frac{N\lambda c_a}{(\mu + N\lambda)E}$$

$$\pi_{11} = \frac{\lambda c_s}{(\mu + N\lambda)E}$$

$$\pi_{12} = \frac{N\lambda^2(c_s + Nc_a)}{\mu(\mu + N\lambda)E}$$

$$\pi_{13} = \frac{N\lambda(1 - c_a)}{\mu E}$$

$$\pi_{14} = \frac{(1 - c_s)}{NE}$$

$$\pi_{15} = \frac{\lambda(1 - c_s)}{\mu E}$$

where

$$E = 1 + \frac{N\lambda c_a}{\beta} + \frac{(1 - c_s)}{N} + \frac{\lambda(N(1 - c_a) + (1 - c_s))}{\mu} + \frac{\lambda(Nc_a + c_s)}{(\mu + N\lambda)} + \frac{N\lambda^2(c_s + Nc_a)}{\mu(\mu + N\lambda)}$$

Therefore the steady-state availability A_{ss} is given by

$$A_{ss} = \frac{1}{E} + \frac{N\lambda c_a}{\beta E} + \frac{\lambda(Nc_a + c_s)}{(\mu + N\lambda)E} + \frac{(1 - c_s)}{NE} \quad (27)$$

Specifically, the steady-state availability model for the Gigabit Route Processor module is

$$A_{ss}(GRP) = \frac{1}{E} + \frac{N\lambda_{grp}c_{agrp}}{\beta_{grp}E} + \frac{\lambda_{grp}(Nc_{agrp} + c_{sgrp})}{(\mu_{grp} + N\lambda_{grp})E} + \frac{(1 - c_{sgrp})}{NE} \quad (28)$$

where

$$E = 1 + \frac{N\lambda_{grp}c_{agrp}}{\beta_{grp}} + \frac{(1 - c_{sgrp})}{N} + \frac{\lambda_{grp}(N(1 - c_{agrp}) + (1 - c_{sgrp}))}{\mu_{grp}} + \frac{\lambda_{grp}(Nc_{agrp} + c_{sgrp})}{(\mu_{grp} + N\lambda_{grp})} + \frac{N\lambda_{grp}^2(c_{sgrp} + Nc_{agrp})}{\mu_{grp}(\mu_{grp} + N\lambda_{grp})}$$

while the steady-state availability model for the IOS Software module is

$$A_{ss}(IOS) = \frac{1}{E} + \frac{N\lambda_{ios}c_{aios}}{\beta_{ios}E} + \frac{\lambda_{ios}(Nc_{aios} + c_{sios})}{(\mu_{ios} + N\lambda_{ios})E} + \frac{(1 - c_{sios})}{NE} \quad (29)$$

where

$$E = 1 + \frac{N\lambda_{ios}c_{aios}}{\beta_{ios}} + \frac{(1 - c_{sios})}{N} + \frac{\lambda_{ios}(N(1 - c_{aios}) + (1 - c_{sios}))}{\mu_{ios}} + \frac{\lambda_{ios}(Nc_{aios} + c_{sios})}{(\mu_{ios} + N\lambda_{ios})} + \frac{N\lambda_{ios}^2(c_{sios} + Nc_{aios})}{\mu_{ios}(\mu_{ios} + N\lambda_{ios})}$$

(v) Clock and Scheduler Card/Switch Fabric Card Model

The Clock and Scheduler Card/Switch Fabric Card module is available when at least four out of five Clock and Scheduler Card/Switch Fabric Card modules are functional. The Continuous Time Markov Chain model of the Clock and Scheduler Card/Switch Fabric Card module is shown in Figure 6. A pair of two numbers m-n represents a state in which m Clock and Scheduler Cards and n Switch Fabric Cards are up.

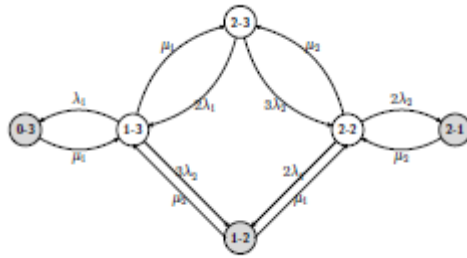


Figure 6 CTMC model for CSC/SFC module.

The steady-state balance equations are obtained as

$$(2\lambda_1 + 3\lambda_2)\pi_{2-3} = \mu_1\pi_{1-3} + \mu_2\pi_{2-2} \quad (30)$$

$$(2\lambda_2 + 2\lambda_1 + \mu_2)\pi_{2-2} = 3\lambda_2\pi_{2-3} + \mu_1\pi_{1-2} + \mu_2\pi_{2-1}$$

$$2\lambda_2\pi_{2-2} = \mu_2\pi_{2-1}$$

$$(3\lambda_2 + \lambda_1 + \mu_1)\pi_{1-3} = 2\lambda_1\pi_{2-3} + \mu_1\pi_{0-3} + \mu_2\pi_{1-2}$$

$$\lambda_1\pi_{1-3} = \mu_1\pi_{0-3}$$

$$(\mu_2 + \mu_1)\pi_{1-2} = 3\lambda_2\pi_{1-3} + 2\lambda_1\pi_{2-2}$$

Hence the steady-state probabilities are given by

$$\begin{aligned}\pi_{2-3} &= \frac{1}{E} \\ \pi_{2-2} &= \frac{3\lambda_2}{\mu_2 E} \\ \pi_{1-3} &= \frac{2\lambda_1}{\mu_1 E} \\ \pi_{0-3} &= \frac{2\lambda_1^2}{\mu_1^2 E} \\ \pi_{2-1} &= \frac{6\lambda_2^2}{\mu_2^2 E} \\ \pi_{1-2} &= \frac{6\lambda_1\lambda_2}{\mu_1\mu_2 E}\end{aligned}$$

where

$$E = 1 + \frac{3\lambda_2}{\mu_2} + \frac{6\lambda_2^2}{\mu_2^2} + \frac{2\lambda_1}{\mu_1} + \frac{2\lambda_1^2}{\mu_1^2} + \frac{6\lambda_1\lambda_2}{\mu_1\mu_2}$$

Therefore the steady-state availability A_{ss} is given by

$$A_{ss} = \frac{1}{E} + \frac{2\lambda_1}{\mu_1 E} + \frac{3\lambda_2}{\mu_2 E} \quad (31)$$

(vi) System Steady-State Availability

Cisco 12000 GSR steady-state availability is given by

$$A_{Cisco} = A_{Upg} \times A_{Cha} \times A_{LC-in} \times A_{LC-out} \times A_{GRP} \times A_{IOS} \times A_{CSC-SFC} \quad (32)$$

Numerical Results

The input parameter values for Cisco 12000 GSR were obtained from Lee (2000) and through discussions with Cisco researchers (Trivedi *et al.*, 2012). The values have been substituted into the closed form solutions of the models in order to compute the steady-state availabilities of the modules of Cisco 12000 GSR as well as the steady-state availability of Cisco 12000 GSR system. Table 5.2 shows the steady-state availabilities of the modules as well as the steady-state availability of Cisco 12000 GSR.

Table 5.2: Steady-state availability of Cisco 12000 GSR and of its modules

Module	Steady-State Availability
Clock Scheduler Card/Switch Fabric Card	0.999999998
IOS	0.999999991
Chassis	0.999998739
Gigabit Route Processor	0.999996701
Line Card-in	0.999954214
Line Card-out	0.999952882
Upgrade	0.999884272
CISCO 12000 GSR	0.99978681

DISCUSSIONS AND CONCLUSIONS

The most available module of Cisco 12000 GSR is the Clock and Scheduler Card/Switch Fabric Card module with a steady-state availability of 0.999999998. This implies that the probability that the Clock and Scheduler Card/Switch Fabric Card module will be functioning is 0.999999998. The probabilities that the IOS, Chassis, Gigabit Route Processor, Line Card-in, Line Card-out and Upgrade modules will be functioning are given by 0.999999991, 0.999998739, 0.999996701, 0.999954214, 0.999952882 and 0.999884272, respectively. The least available module is the Upgrade module with a steady-state availability of 0.999884272. The overall steady-state availability of Cisco 12000 GSR system is 0.99978681.

In analysis, the redundancy of the modules is considered. The Chassis and Upgrade modules are non-redundant modules. Actually, one of the assumptions of the study of Cisco 12000 GSR system is that an upgrade of the system causes outage of the whole system. The upgrade module is the least available, whenever the system undergoes upgrading it is totally shut down. System upgrades result in the greatest downtime hence more research should be conducted on how to reduce Cisco 12000 GSR system upgrade time spans. Though the Chassis module is also non-redundant, it is the third most available module at a functional probability of 0.999998739. Both the Line Card-in and the Line Card-out modules are also non-redundant and are fifth and sixth most available modules with functional probabilities of 0.999954214 and 0.999952882, respectively. More research needs to be conducted in order to improve on the steady-state availabilities of the non-redundant Chassis, Line Card-in and Line Card-out modules. The Gigabit Route Processor and the IOS software modules are 1: N redundant modules with fault coverage and switch-over factors. The IOS software module is the second most available module with a probability of 0.999999991 of functioning and the Gigabit Route Processor is the fourth most available module at 0.999996701. The steady-state availabilities of these two modules can be increased by having more standby units, improving on the coverage and switch-over factors

and by increasing the repair rates. The Clock and Scheduler Card/Switch Fabric Card module is the most available at 0.999999998 and is operational as long as four-out-of-five modules are operational. The steady-state availability of the Clock and Scheduler Card/Switch Fabric Card module can be improved by increasing the repair rates while more research can be conducted in order for the module to be operational with fewer than four-out-of-five modules being functional. Finally, the steady-state availability of the Cisco 12000 GSR system stands at a probability of 0.99978681. The steady-state availability of the system can be increased by improving on the individual module steady-state availabilities as has been suggested.

In conclusion the steady-state availability of Cisco 12000 GSR is 0.99978681. The most available module of Cisco 12000 GSR is the Clock and Scheduler Card/Switch Fabric Card module with a functional probability of 0.999999998.

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Uncertainty Analysis of the Availability of Cisco 12000 GSR

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ABSTRACT: Stochastic models are appropriate for modelling and analysing the dependability of critical systems. The dependability attributes include availability, reliability, safety, integrity, maintainability, survivability, performance and confidentiality. Stochastic models are useful for estimating the output measures of interest of the critical systems. Generally, fixed input parameter values are used in the models to estimate the output measures of interest but the input

parameter values have incomplete information or are obtained from expert guesses. Hence the input parameter values have uncertainty, called epistemic uncertainty, associated with them. The output measures of interest depend upon the input parameter values used implying that the output measures of interest have uncertainty associated with them. Of paramount importance to the users of critical systems are the levels of uncertainty associated with the estimates of the output measures of interest. In this paper, the uncertainty in the computation of the steady-state availability of Cisco 12000 Gigabit Switch Router is presented. A novel uncertainty propagation wrapper is used for the uncertainty analysis.

Keywords: Uncertainty analysis, Epistemic uncertainty, Uncertainty propagation wrapper, Output measure of interest, Input parameters.

INTRODUCTION

Stochastic models are useful for modelling and analysing the dependability of critical systems. The dependability attributes include availability, reliability, safety, integrity, maintainability, confidentiality (Avizienis *et al.*, 2004), survivability and performance (Trivedi *et al.*, 2009). Generally, random behaviour exists in the systems being modelled or in the environments in which the systems operate. The natural randomness in the systems is referred to as aleatory uncertainty. Stochastic models which capture the randomness in the systems being modelled are useful for estimating the output measures of interest. Fixed input parameter values are used in the models to estimate the output measures of interest but the input parameter values have incomplete information or are obtained from expert guesses. Hence the input parameter values have uncertainty, called epistemic uncertainty, associated with them. The output measures of interest depend upon the input parameter values used, implying that the output measures of interest are conditional on the input parameter values used (Sinpurwalla, 2006). Hence the output measures of interest have uncertainty associated with them. Of paramount importance to the users of critical systems are the levels of uncertainty associated with the estimates of the output measures of interest.

In a case study of the IBM SIP SLEE application server cluster system (Mishra and Trivedi, 2011), uncertainty propagation method was used to compute the confidence interval for the system availability. A three-level hierarchical model of the IBM SIP SLEE application server cluster system was used. Fault Trees were used for the system and sub-system levels while a Markov Chain model was used for the failure-repair behaviour of individual hardware or software components. The entire hierarchical model had sixty-three input parameters. SHARPE (Trivedi and Sahner, 2009) was used to solve the hierarchical aleatory model. The uncertainty propagation was performed using the Latin Hypercube sampling procedure and the uncertainty propagation wrapper was implemented in Mathematica (Wolfram Mathematica 6, 2007). The two-sided 95 per cent confidence interval for the availability of IBM SIP SLEE cluster system was found to be (0.99999509, 0.99999649).

Mishra and Trivedi (2011) further present a second case study on which the uncertainty propagated through a service reliability and performance model of a composite web service called Travel-Agent was performed. A Continuous Time Markov Chain model of the composite web service was developed. The aleatory model outputs were evaluated using Mathematica (Wolfram Mathematica 6, 2007). Again, the uncertainty propagation was performed using the Latin Hypercube sampling procedure and the uncertainty propagation wrapper was implemented in Mathematica. The two-sided 95 per cent confidence interval of the mean service response time of the composite web service was found to be (7.6730, 8.3856) while the two-sided 95 per cent confidence interval of the reliability of the composite web service was computed as (0.92217, 0.97759).

In a related study (Mishra and Trivedi, 2012), uncertainty propagation method was used to compute the confidence interval of the reliability of the NASA Remote Exploration and Experimentation system. A three-level hierarchical model captured the failure behaviour of both the system and the system components. At the lowest level, a Markov model captured the failure behaviour of the software sub-system, in the middle level the failure behaviour of the individual components were captured using Reliability Block Diagrams while the top-level model was a Fault Tree which provided the overall system reliability. The hierarchical model was solved using SHARPE (Trivedi and Sahner, 2009). Uncertainty propagation was performed using the Latin Hypercube sampling procedure and the uncertainty propagation wrapper was implemented in Mathematica (Wolfram Mathematica 6, 2007). The two-sided 95 per cent confidence interval for the reliability of the Remote Exploration and Experimentation system was found to be (0.949485, 0.981994).

In the IBM BladeCenter system case study (Devaraj *et al.*, 2010) a Monte Carlo sampling based method for propagating the epistemic uncertainty through the system availability model was used. Uncertainty propagation of the confidence interval for each of the model input parameters was performed in order to obtain the confidence interval of the system availability. A hierarchical model of the availability of the IBM BladeCenter system consisted of a Fault Tree at the top level while the subsystems were modelled as Markov Chains. The system availability model was solved using SHARPE (Trivedi and Sahner, 2009). The 95 per cent two-sided confidence intervals of the availability of the BladeCenter system were obtained for different numbers of stand-by Blade Servers. Hence for 0, 1, 2, 5, 8 and 11 stand-by Blade Servers, the 95 per cent two-sided confidence intervals were (0.9991384, 0.9993499), (0.9999972, 0.9999985), (0.9999975, 0.9999988), (0.9999975, 0.9999988), (0.9999979, 0.9999988) and (0.9999979, 0.9999988), respectively.

In this paper the uncertainties in the computations of the steady-state Availability of Cisco 12000 Gigabit Switch Router in (Musiga, 2016) are presented.

THE MODEL

As noted earlier, the output measures of interest are conditional on the input parameter values used hence the output measure of interest need to be Unconditioned. By applying the theorem of total probability (Trivedi, 2001), unconditioning of the model output measure of interest is performed by multi-dimensional integration of the epistemic distributions of the random variables of the model input parameters.

In a stochastic model, the input parameters form a random vector $\{\Lambda_i, i = 1, 2, \dots, l\}$. This implies that the output measure M is a function of the l input parameters, that is, $M = g(\Lambda_1, \Lambda_2, \dots, \Lambda_l)$. When the output measure of interest is computed using fixed input parameter values, then the measure of interest, denoted by $M(\cdot)$, is conditional on the input parameter values used (Sinpurwalla, 2006). Using the theorem of total probability (Trivedi, 2001), this is unconditioned by multiple integration to obtain the unconditional expected value of the output measure of interest M by using the joint epistemic density $f_{\Lambda_1, \Lambda_2, \dots, \Lambda_l}(\lambda_1, \lambda_2, \dots, \lambda_l)$, denoted by $f(\cdot)$, of the parameters as random variables, hence

$$E[M] = \int \dots \int M(\cdot) f(\cdot) d\lambda_1 \dots d\lambda_l \quad (1)$$

and the second moment of the output measure of interest M is given by

$$E[M^2] = \int \dots \int (M(\cdot))^2 f(\cdot) d\lambda_1 \dots d\lambda_l \quad (2)$$

hence

$$Var[M] = E[M^2] - (E[M])^2 \quad (3)$$

The type and parameters of the epistemic distributions to be used in Equations (1), (2) and (3) from the observed values of times to failure need to be determined. The epistemic random variables are assumed to be independent thus the joint probability density functions are factored into the product of the marginal probability density functions.

Bayes' Theorem

Let $X_1, X_2, \dots, X_k$ be independent and identically distributed random variables used to compute the joint estimate of the parameter of the observed time to failure X of a component. Then the epistemic probability density function of PM QU_TE Λ_i given the observed values and using the continuous form of Bayes' Theorem (Trivedi, 2001) is given by

$$59 \quad (<)$$

where $f_{\Lambda_i}(\lambda_i)$ is the prior density function which attributes uncertainty to a quantity and $f_{\Lambda_i|x_1, x_2, \dots, x_k}(\lambda_i|x_1, x_2, \dots, x_k)$ is the epistemic posterior probability density function. The times to failures, repairs and recovery actions are exponentially distributed hence it is necessary to determine

the epistemic distribution for the rate parameter of the exponential distribution.

Epistemic PDF for Exponential Distribution

If S , the time to failure of a component is given by $S = X_1 + X_2 + \dots + X_k$ where Λ is the model parameter, then the random variable S given by

$$S = X_1 + X_2 + \dots + X_k = \sum_{i=1}^k X_i \quad (5)$$

is k-stage Erlang distributed with parameter λ , (Trifedi, 2001). Hence the probability density function of S given Λ is

$$f_{S|\Lambda}(s|\lambda) = \frac{\lambda^k s^{k-1} e^{-s\lambda}}{(k-1)!} \quad (6)$$

By Bayes' theorem, the posterior density of λ is given by

$$f_{\Lambda|S}(\lambda|s) = \frac{f_{\Lambda}(\lambda) f_{S|\Lambda}(s|\lambda)}{\int_0^{\infty} f_{\Lambda}(\lambda) f_{S|\Lambda}(s|\lambda) d\lambda} \quad (7)$$

where $f_{\Lambda}(\lambda)$ is the prior density of λ . Using Jeffreys' prior of Λ as $f_{\Lambda}(\lambda) = \frac{s}{\lambda}$, [3], then

$$f_{\Lambda|S}(\lambda|s) = \frac{s^k \lambda^{k-1} e^{-\lambda s}}{(k-1)!} \approx \text{Erlang}(k, s) \quad (8)$$

is k-stage Erlang with rate parameter s . This is the epistemic probability density function for the rate parameter Λ when the aleatory probability density function is exponential.

Epistemic PDF for Bernoulli Distribution

Suppose that the input parameter Λ is a coverage or detection parameter obtained from a fault-injection experiment where k faults are introduced. Let the random variable Y be the number of successfully covered faults, then Y is binomial (k, λ) thus

$$p_{Y|\Lambda}(y|\lambda) = \binom{k}{y} \lambda^y (1-\lambda)^{k-y} \quad (9)$$

then the probability distribution function of $f_{\Lambda|Y}(\lambda|y)$ is defined as

$$f_{\Lambda|Y}(\lambda|y) = \frac{\Gamma(k+2)}{\Gamma(y+1)\Gamma(k-y+1)} \lambda^y (1-\lambda)^{k-y} \quad (10)$$

using the non-informative Jeffreys' flat prior of $f_{\Lambda}(\lambda) = 1$ [3], then

$$f_{\Lambda|Y}(\lambda|y) = \frac{\Gamma(k+2)}{\Gamma(y+1)\Gamma(k-y+1)} \lambda^y (1-\lambda)^{k-y} \quad (11)$$

This is the epistemic probability distribution function for the parameter Λ when the aleatory probability distribution function is Bernoulli.

Sample Size from Epistemic Distribution

Since the parameters were assumed to be independent random variables, samples are drawn from each of the epistemic distributions. The point estimate is given by

$$\hat{\lambda} = \frac{k}{S}$$

where k is the number of failures observed and S is the value of the accumulated life on test. Consideration is given to the number of observations that is to be used to compute the point estimate of Each model input parameter Λ_i . The sample size to be drawn from the epistemic distribution of each of the model input parameters is $n = \{\max(k_i)\}$. Samples of size n are then generated from the l model input parameter epistemic distributions resulting in a vector of parameter values as shown in matrix form in equation (12).

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} \lambda_{11} & \lambda_{21} & \dots & \lambda_{l1} \\ \lambda_{12} & \lambda_{22} & \dots & \lambda_{l2} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{1n} & \lambda_{2n} & \dots & \lambda_{ln} \end{pmatrix} \quad (13)$$

$$\text{QUOTE} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} \lambda_{11} & \lambda_{21} & \dots & \lambda_{l1} \\ \lambda_{12} & \lambda_{22} & \dots & \lambda_{l2} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{1n} & \lambda_{2n} & \dots & \lambda_{ln} \end{pmatrix} \quad (12) \quad \text{The output measure is}$$

computed from each of the n samples yielding the set of output measures in the form

Unce2uainty Propagation Wrappdr

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to declare a variable with the following syntax is used;

`[conf,vcr-name,var-value,conf-level,half-width/coverage-lower,erlang/beta]`

where *var-name* represents the variable name, *var-value* represents the value of the variable, *conf-level* indicates the confidence level, *half-width* represents the half-width of the variable, *coverage-lower* represents the lower limit of the variable, *erlang* indicates that the variable follows an Erlang distribution and *beta* indicates that the variable follows a Beta distribution. To indicate the output metric for which uncertainty analysis needs to be performed, "expected" and "variance" are included before the "expr" command. The uncertainty propagation wrapper then extracts the required parameters from the SHARPE (Trivedi and Sahner, 2009) input file and uses the acquired data to generate sample points after which the system is evaluated at the generated sample points. The output of the system at the sample points are stored and statistical analysis is performed on the points to find the "expected" and the "variance" of the output metric being analysed. A flowchart indicating the work flow of the software is shown in Figure 1.

APPLICATION

In this section the uncertainty propagation method is illustrated using the steady-state availability computed for Cisco 12000 Gigabit Switch Router (GSR). A brief overview of the system description is provided. The Cisco 12000 GSR comprises seven sub-systems or modules; Upgrade, Line Card-in, Line Card-out, Clock and Scheduler Card/Switch Fabric Card, Gigabit Route Processors, Chassis and Cisco IOS modules. The Gigabit Route Processors, IOS and Clock and Scheduler Card/Switch Fabric Card are modules with redundancy. The top level hierarchical model of the system is a block diagram while the lower level models of the modules are Continuous Time Markov Chains. Times to failure and repair are exponentially distributed and coverage and switch-over factors are incorporated in the models where applicable. In the next subsection, the algorithm followed using the uncertainty propagation wrapper is explained.

Uncertainty Propagation

Uncertainty propagation software (Upadhyaya, 2014) is used to compute the uncertainty propagated through the stochastic models of the system modules. To calculate the uncertainty in the output metrics the required parameters are extracted from the SHARPE (Trivedi and Sahner, 2009) input file and using the acquired data, sample points are generated and the system is evaluated at those sample points. The output of the system at these points is stored and statistical analysis is performed on these points to find the expected and the variance of the output metric being analysed. The stochastic steady-state availability metrics for the system modules were obtained in (Musiga, 2016). The input parameter values for Cisco 12000 GSR were obtained from (Lee, 2000) and through discussions with Cisco researchers (Trivedi et al., 2012). The uncertainties computed for each run are shown in Table 1.

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DISCUSSIONS(AND CONCLUSIONS

A summary of the steady-state availability of Cisco 12100 GSRs was computed in [Mu3iga, 2016\ and the variance computed for the individual modules using the uncertainty propagation wrapper are presented in Table 1.

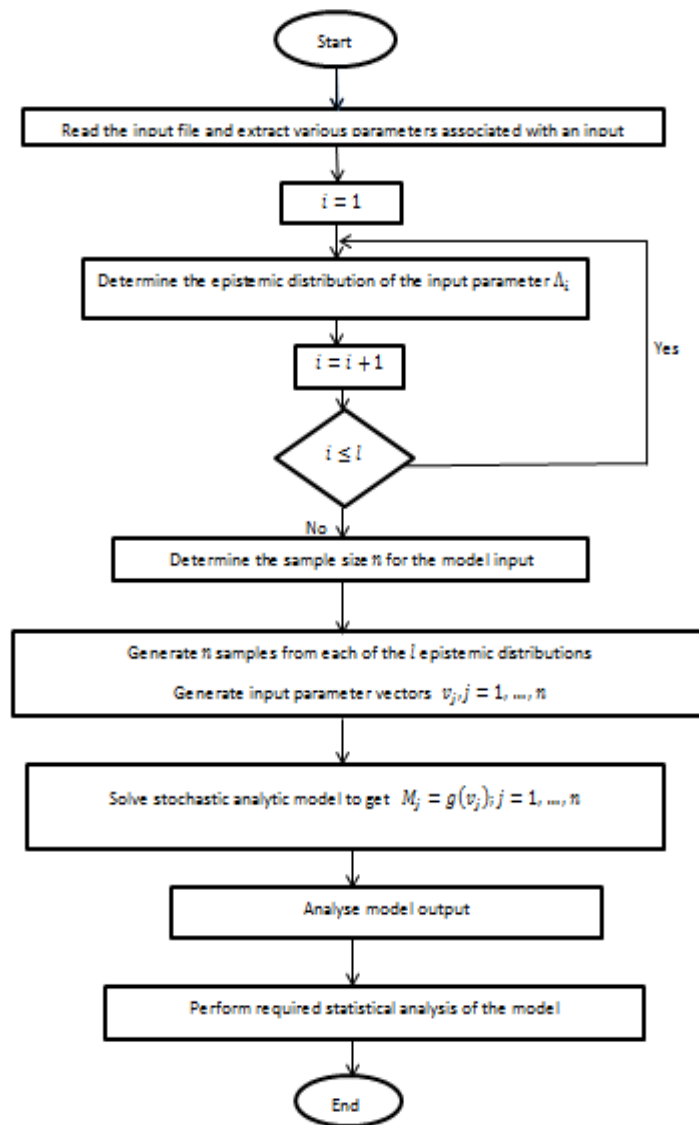


Figure 1.QncerTainty Propagation wrapper flOwcharT.

Table !: Steady-state availabilities and variances of steady-state availabilities of the modules of Cisco 12800 GSR.

Module	Steady-State Availability	Variance
Clock Scheduler Card/Switch Fabric Card	0.999999998	0.000050
IOS	0.999999991	0.002486
Chassis	0.999998739	0.000005
Gigabit Route Processor	0.999996701	0.017361
Line Card-in	0.999954214	0.000043
Line Card-out	0.999952882	0.000045
Upgrade	0.999884272	0.000005

The modules with large variances are the Gigabit Route Processor and IOS software modules at variances of 0.017361 and 0.002486, respectively. The two modules have two types of input parameter values each, the rate input parameters and the coverage and switch-over factor input parameters, leading to the lower uncertainty values.

The standard deviation values for the uncertainty of each of the modules and the range values within which the steady-state availability of the modules of Cisco 12000 GSR lie are shown in Table 2. Hence the steady-state availability of the Clock and Scheduler Card/Switch Fabric Card module lies between 0.999928998 and 1, the steady-state availability of the IOS software module lies between 0.999928991 and 1, the steady-state availability of the Chassis module lies between 0.997762671 and 1, the steady-state availability of the Gigabit Route Processor module lies between 0.992925701 and 1, the steady-state availability of the Line Card-in module lies between 0.993396775 and 1, the steady-state availability of the Line Card-out module lies between 0.993244678 and 1 and the steady-state availability of the Upgrade module lies between 0.997648272 and 1. In conclusion, the steady-state availability of Cisco 12000 GSR lies between 0.804502004 and 1.

Table 2: Range of values for the steady-state availabilities of Cisco 12000 GSR

Module	Steady-state Availability	Variance	Std. Deviation	Range of Values
CSC/SFC	0.999999998	0.000050	0.007071	0.992928998 - 1.000000000
IOS	0.999999991	0.002486	0.049860	0.950139991 - 1.000000000
Chassis	0.999998739	0.000005	0.002236	0.997762671 - 1.000000000
Gigabit Route Processor	0.999996701	0.017361	0.131761	0.868235701 - 1.000000000
Line Card-in	0.999954214	0.000043	0.006557	0.993396775 - 1.000000000
Line Card-out	0.999952882	0.000045	0.006708	0.993244678 - 1.000000000
Upgrade	0.999884272	0.000005	0.002236	0.997648272 - 1.000000000
Cisco 12000 GSR	0.99978681	0.038136	0.195284	0.804502004 - 1.000000000

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The Effects of Intermolecular Interactions in Line Broadening Phenomena

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ABSTRACT: We describe the time evolution of a system when the molecules are perturbed with an external field at temperature T . The system under investigation is a gas in a microscopic state described by a density matrix. It is shown that at high collision frequencies one needs stronger impressed fields in order to reorient the particles. We apply single relaxation theories characterized by a time between collisions.

INTRODUCTION

In the present communication we shall as in the past (Malo, 2005; Malo, 1995a; 1995b) limit our consideration to linear molecules of moment of inertia I and linear response of the system to the applied field. The N -particle density matrix obeys the usual kinetic equation of the form

$$\frac{\partial \rho^{(1)}}{\partial t} + \frac{i}{h} [H^{(N)} \rho^{(N)}] = \frac{\delta \rho(t)}{\delta t} \quad (1)$$

where N is the number of particles in the gas and $H^{(N)}$ is the N -particle Hamiltonian assumed to be of the form

$$H^{(N)} = \sum_{i=1}^N H_i^{(1)} + \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (2)$$

$\frac{\delta \rho}{\delta t(t)}$ is the collision term and $H_i^{(1)}$ is the one-particle Hamiltonian-kinetic energy, and V_{ij} is the short range intermolecular potential between molecules i and j and is responsible for molecular collisions.

By assuming however that H is a time-constant Hamiltonian, the reservoir will drag the system to a canonical distribution in which the density matrix tends to $\rho_{eq}(t)$ representing the equilibrium density matrix in accordance with Boltzmann law appropriate to the instantaneous value of the time dependent Hamiltonian $H(t)$

$$H(r,t) = \sum_i H_i^{(t)} + \frac{1}{2} \sum_{i \neq j} V_{ij} + \sum_k U_k(t)$$

where $U = \mu E(t)$ is the impressed field component of the Hamiltonian and μ is the dipole moment operator.

For a linear molecule in an external field along the polar axis, μ_z is diagonal in coordinate representation (Malo, 1976; Gross and Malo, 1972) and has the value $\mu \cos \theta$. Thus the density matrix equation involving $H(r,t)$ is very difficult to solve exactly except in a very formal manner. This is so because it has a great number of degrees of freedom. However, on the assumption that the gas under study is sufficiently dilute, several approximations can be made in order to obtain an approximate solution to this equation (Xuan and Mchale, 1998). The fundamental assumption here is that in a dilute gas, the molecules are far apart most of the time and consequently are independent of each other. This is really a statement of the Boltzmann property which simply says that the N -particle density matrix is a product of one-particle density matrices. The above property is assumed to hold anywhere in the gas except where two or more molecules are colliding. For sufficiently dilute gas, the number of molecules that are colliding at any one instant of time is very small such that the Boltzmann property should hold anywhere (Novikov *et al.*, 2001). However, because of the intermolecular potential V_{ij} , the molecules do in fact collide and this no doubt has an effect on the single particle density matrix (Felker, 2006).

The immediate effect of intermolecular interactions is that it will hinder the drift motion of the individual molecules but on the contrary enhance their collective motion [Kola and Luo, 2007] thus the cumulative effect of the interactions is to increase total polarization of the system as a whole. Since absorption will thus increase for a given collision frequency, the line width will become broadened (Beeken, and Lischka, 2005). The most direct method for studying the effects of intermolecular potentials between molecular systems that do not form stable compounds under ordinary conditions is the molecular beam scattering experiment (MBSE) (Komatsu and Nakagawa, 2008). However, for studying effects of intermolecular potentials of systems that form stable compounds, the beam scattering method cannot compete with the optical spectroscopy which to a large extent will only give information on the attractive portion of the potential. It should be noted that the beam scattering method is more universal and covers the entire energy range (Xu *et al.*, 1988). Intermolecular potentials are of basic importance for the understanding of many macroscopic properties of matter. Our final task lies in the computation of the expectation value of the dipole moment operator – Polarization.

EXTERNAL FIELD RESPONSE

The N -particle density matrix satisfies the operator equation given by the expression (1) where the LHS is the quantum analog of the Liouville's equation and so describes the variation of the

density matrix caused by the time dependent Hamiltonian and the RHS gives effect of interaction–collision term.

The Hamiltonian consists of a free particle $H_i^{(1)}$ and V_{ij} the interaction of the permanent dipoles with an external field $E(t)$. The effect of interaction $\frac{\delta\rho}{\delta t}$ can be given several expressions depending on the types of systems under consideration (Malo, 1995b). We shall however limit our study to (K-S) (Malo, 1976) and (G-L) (Gross and J.O. Malo, 1972) models of the collision term. The Brownian motion model will be presented in a later communication.

A. Karplus – Schwinger Model (K-S)

In this model, the collision term takes the form

$$\frac{\delta\rho^{(N)}}{\delta t} = -\frac{1}{\tau}(\rho^{(N)} - \rho_{eq}^{(N)}(t)) \quad (3)$$

This is a single relaxation theory characterized by a time τ between collision [Malo, 1995b; Malo, 1976]. Since we are only interested in linear response to the applied field, the impressed field term will vanish. It is convenient to introduce deviation.

$$D^{(1)}(t) = \rho^{(1)} - \rho_{eq^{(1)}}(t) \quad (4)$$

and equation (3) immediately takes the form

$$\frac{\partial D^{(1)}}{\partial t} + \frac{D^{(1)}}{\tau} + \frac{i}{h} \left[\sum_i H_i \left(\frac{1}{i} \right) D^{(1)} \right] + \frac{i}{2h} \left[\sum_{i=j} V_{ij} D^{(2)} \right] = -\frac{\partial \rho_{eq}^{(1)}}{\partial t} \quad (5)$$

The above equation can be handled in a number of ways by using trace algebra. In energy representation it has the form

$$\left(\frac{\partial}{\partial t} + i\omega_{\ell\ell} + \frac{1}{\tau} \right) \langle \ell m / D^{(1)} / \ell' m' \rangle = - \langle \ell m \left| \frac{\partial \rho_{eq}^{(1)}}{\partial t} \right| \ell' m' \rangle - \frac{i}{h} \langle \ell m \left| \left[\sum_{i \neq j} V_{ij}^{(2)} \right] \right| \ell' m' \rangle \quad (6)$$

where $\omega_{\ell\ell'} = \frac{E_{\ell} - E_{\ell'}}{h}$ is the angular frequency associated with transition $\ell \rightarrow \ell'$ of the unperturbed system. The last term involving intermolecular interactions can be written in the form

$$\sum_{\substack{nk \\ n'k'}} \left\{ \langle \ell m | nk \rangle \langle nk | V | n'k' \rangle D^{(2)} | n'k' \rangle \langle n'k' | \ell' m' \rangle \right. \\ \left. - \langle \ell m | nk \rangle \langle nk | D^{(2)} | n'k' \rangle V | n'k' \rangle \langle n'k' | \ell' m' \rangle \right\} \quad (7)$$

The first term thus corresponds to the non-degenerate internal states $\langle nk | V | n'k' \rangle$ with respect to the energy due to intermolecular forces and the second term corresponds to the degenerate internal states $\langle n'k' | V | n'k' \rangle$.

A(i) Non-degenerate Case

In sharp contrast to the degenerate case, the internal state wave function for a free particle contains only one possible state and the corresponding density matrix will be diagonal in internal states $\langle m'k' | D^{(1)} | \ell' m' \rangle$.

Thus equation (6) will take the form

$$\left(\frac{\partial}{\partial t} + \omega_{\ell\ell'} + \frac{1}{\tau} \right) \langle \ell m | D^1 | \ell' m' \rangle = - \langle \ell m | \frac{\partial \rho e q^{(1)}}{\partial t} | \ell' m' \rangle \\ - \frac{i}{2h} \sum_{\substack{n \neq k \\ n' \neq k'}} \langle \ell m | nk \rangle \langle nk | V | n'k' \rangle \langle n'k' | D^{(2)} | n'k' \rangle \langle n'k' | \ell' m' \rangle \quad (8)$$

The expressions above can further be reduced into coordinate representation by multiplying to the left $\langle \theta' \phi' | \ell m \rangle$ and to the right $\langle \ell' m' | \theta' \phi' \rangle$ and we obtain the following integral equation

$$\langle \theta' \phi' | D^{(1)} | \theta' \phi' \rangle = - \sum_{\substack{\ell m \\ \ell' m'}} \frac{1}{\Delta_{\ell\ell'}} \left\{ \langle \theta' \phi' | \ell m \rangle \langle \ell m | \frac{\partial \rho e q^{(1)}}{\partial t} | \ell' m' \rangle \langle \ell' m' | \theta' \phi' \rangle \right. \\ \left. + \int K_1(\cos \alpha) \sin \alpha d\theta \phi \langle \theta \phi | D^{(2)} | \theta \phi \rangle \right\} \quad (9)$$

where

$$K_1(\cos \alpha) = \frac{4\pi}{2\tau} \sum_{\substack{n \neq K \\ n' \neq K' \\ \ell \ell'}} \frac{1}{\Delta_{\ell\ell'}} \langle nk | V | n'k' \rangle \frac{2\ell+1}{4\pi} \frac{2\ell'+1}{4\pi} \cdot P_{\ell}(\cos \alpha) P_{\ell'}(\cos \alpha)$$

$$\Delta_{\ell\ell'} = \frac{\partial}{\partial t} + i\omega_{\ell\ell'} + \frac{1}{\tau}$$

A(ii) Degenerate Case

For this case, we need in general a Wigner distribution density matrix which is a distribution in position – momentum space and a density matrix in internal state space. This is necessary for the degenerate case since internal states of the system may be any linear combination of the degenerate internal states. Carrying out the same type of calculations as in the non-degenerate case, we come to the final integral equation of the form.

$$\begin{aligned} \langle \theta\phi | D^{(2)} | \theta'\phi' \rangle = & - \sum_{\ell m} \frac{1}{\Delta_{\ell\ell'}} \langle \theta'\phi' | \ell m \rangle \langle \ell m | \frac{\partial \rho_{eq}^{(1)}}{\partial t} | \ell m' \rangle \langle \ell m' | \theta'\phi' \rangle \\ & + \int K_2(\cos\alpha) \sin\alpha d\alpha d\phi \sin\theta' d\theta' d\phi' \langle \theta\phi | D^{(2)} | \theta'\phi' \rangle \end{aligned} \quad (10)$$

where

$$K_2(\cos\alpha) = \frac{4\pi}{2\tau} \sum_{\substack{n=k \\ n'=k' \\ e\ell}} \frac{1}{\Delta_{\ell\ell'}} \langle n'k' | V | n'k' \rangle \cdot \frac{2\ell+1}{4\pi} \cdot \frac{2\ell'+1}{4\pi} P_{\ell'}(\cos\alpha) P_{\ell}(\cos\alpha)$$

B. Gross – Lebowitz Model (G – L)

In this model, the effect of interaction takes the form

$$\frac{\delta \rho^{(1)}}{\delta t} = \frac{\rho^{(1)}(\theta\phi)}{\tau} + \frac{\rho_{eq}^{(1)}(\theta\phi)}{2\tau} \left[\frac{\rho^{(1)}(\theta\phi)}{\rho_{eq}^{(1)}(\theta\phi)} + \frac{\rho^{(1)}(\theta^1\phi^1)}{\rho_{eq}^{(1)}(\theta^1\phi^1)} \right]$$

This is still a single relaxation time characterized by a time τ between collisions. Further on we shall denote

$$\frac{\rho^{(1)}(\theta\phi)}{\rho_{eq}^{(1)}(\theta\phi)} + \frac{\rho^{(1)}(\theta^1\phi^1)}{\rho_{eq}^{(1)}(\theta^1\phi^1)} = R$$

The bracket is symmetric in order to maintain character of the collision term in the course of time. Thus equation (1) will take the form

$$\frac{\partial \rho^{(1)}}{\partial t} + \frac{i}{h} \left[\sum_i H_i^{(1)} \rho^{(1)} \right] + \frac{i}{2h} \left[\sum_{j \neq i} V_{ij} p(2) \right] + \frac{i}{h} \left[\sum_K V_K \rho^{(1)} \right] = -\frac{\rho^{(1)}}{\tau} + \frac{\rho_{eq}^{(1)}}{2\tau} R \quad (11)$$

And again limiting our consideration to linear response to the applied field the fourth term on the LHS will vanish. We could then write equation (11) in a more explicit form for the three dimensional rigid rotator. Introducing deviation via equation (4)

$$\frac{\partial D^{(1)}}{\partial t} + \frac{i}{h} \left[\sum_i H_1^{(1)} D^{(1)} \right] = - \frac{\partial \rho_{eq}^{(1)}}{\partial t} - \frac{D^{(1)}}{\tau} + \frac{i}{2h} [V_{12} D^{(2)}] \\ + \frac{4\pi}{2} \{ \langle \theta\phi | D^{(1)} | \theta\phi \rangle \langle \theta\phi | \rho_{eq}^{(1)} | \theta\phi \rangle + \langle \theta'\phi' | \rho_{eq}^{(1)} | \theta'\phi' \rangle \langle \theta'\phi' | D^{(1)} | \theta'\phi' \rangle \} \quad (12)$$

The above equation can be handled in exactly the same way as that for the non-degenerate case (8) by moving into energy representation and back again into coordinate representation. Thus we finally obtain the following integral equations for:

B(i) Non-degenerate case

$$\langle \theta'\phi' | D^{(1)} | \theta'\phi' \rangle = \int M_1(\cos\alpha) \sin\theta d\theta d\phi \langle \theta\phi | D^{(2)} | \theta\phi \rangle \\ + \sum_{\substack{\ell m \\ \ell' m'}} \frac{1}{\Delta_{\ell\ell'}} \langle \theta'\phi' | \ell m \rangle \langle \ell m | \frac{\partial \rho_{eq}^{(1)}}{\partial t} | \ell' m' \rangle \langle \ell' m' | \theta'\phi' \rangle \quad (13)$$

where

$$M_1(\cos\alpha) = \frac{4\pi}{2\tau} \sum_{\substack{n \neq k \\ n' \neq k' \\ e e'}} \frac{1}{\Delta_{\ell\ell'}} \{ \exp(-\beta E_{\ell'}) - \langle nk | V | n'k' \rangle \} \cdot \frac{2\ell+1}{4\pi} \frac{2\ell'+1}{4\pi} P_{\ell}(\cos\alpha) P_{\ell'}(\cos\alpha)$$

B(ii) Degenerate Case

$$\langle \theta\phi | D^{(1)} | \theta'\phi' \rangle = M_2(\cos\alpha) \sin\theta\phi \theta d\phi \sin\theta'd\theta'd \langle \theta\phi | D^{(2)} | \theta'\phi' \rangle$$

$$+ \sum_{\substack{\ell m \\ \ell' m'}} \frac{1}{\Delta_{\ell \ell'}} \langle \theta \phi | \ell m \rangle \langle \ell m | \frac{\partial \rho_{eq}^{(1)}}{\partial t} | \ell' m' \rangle \langle \ell' m' | \theta' \phi' \rangle \quad (14)$$

where

$$M_2(\cos \alpha) = \frac{4\pi}{2\tau} \sum_{\substack{n \neq k \\ n' \neq k' \\ \ell \ell'}} \frac{1}{\Delta_{\ell \ell'}} \{ \exp(-E_\ell) - \langle nk | V | nk \rangle \} \cdot \frac{2\ell+1}{4\pi} \cdot \frac{2\ell'+1}{4\pi} P_\ell(\cos \alpha) P_{\ell'}(\cos \alpha)$$

Solution of Integral Equations

a) Karplus – Schwinger Model

The integral equations derived in section 2 are coupled equations. In the case of linear response to the impressed fields, the corresponding kinetic equation for the pair density matrix $\langle \theta \phi | D^{(2)} | \theta \phi \rangle$ can be given an approximate solution if triplet collisions are neglected. For expression $\langle \theta \phi | D^{(2)} | \theta \phi \rangle$ we shall insert this on the right hand side of equation (7) and obtain a generalized (non-Markovian) integro-differential kinetic equation for the single density matrix-deviation $D^{(1)}$. Equation (9) will thus take the form

$$\begin{aligned} \langle \theta' \phi' | D^2 | \theta' \phi' \rangle &= \sum_{\substack{\ell m \\ \ell' m'}} \Delta_{\ell \ell'}^{-1} \langle \ell m \rangle \langle \ell m | \frac{\partial \rho_{eq}^{(1)}}{\partial t} | \ell' m' \rangle \langle \ell' m' | \theta' \phi' \rangle \\ &- \sum_{\ell \ell'} \Delta_{2\ell \ell}^{-1} \int K_1(\cos \alpha) \sin \theta d\theta d\phi i\omega \langle \theta \phi | \rho_{eq}^{(1)} | \partial \theta \rangle \end{aligned} \quad (15)$$

where

$$\Delta_{2\ell \ell'} = i\omega \frac{1}{\tau} + i\omega_{\ell \ell'} + B(\theta \phi) \text{ for steady state solutions.}$$

From the Boltzmann property

$$\rho_{eq}^{(N)} = \prod_{i=1}^N \rho_{eq}^{(1)}(1)$$

The integral term can be written as follows:-

$$\sum_{\ell\ell} i\omega \Delta_2^{-1} \int K_1(\cos\alpha) \sin\theta d\theta < \theta\phi | \rho_{eq}^{2(1)} | \theta\phi >.$$

The first term on the RHS of equation (15) gives the usual K-S result is familiar from previous works [1]. The second term results in modification to the absorption coefficient.

Let us write the integral Kernel in explicit energy notations.

$$K_1(\cos a) = \frac{4\pi}{2\tau} \sum_{\substack{nk \\ n'k' \\ \ell\ell'}} \Delta_{\ell\ell}^{-1} < nk | V_{12} | n'k' > \frac{2\ell'+1}{4\pi} \cdot P_\ell(\cos a) P_{\ell'}(\cos a) \quad (16)$$

In analyzing the integral term which is responsible for the effects of intermolecular interactions, we use the author's previous works (Malo, 2005; Malo, 1995a) and after some calculations and rearrangements, we come to the following expression for the contribution.

$$V_+(\ell\ell') = -\frac{i\omega}{2\tau} \mu^2 \Delta_{\ell\ell}^{-1} < \ell m | V | \ell' m' > \{2L\}^2 \quad (17)$$

$$L = \sum_{\ell}^n \frac{\exp(-b\ell^2)}{[\ell^2 + (c + i\omega_1)^2]}$$

The revised K-S is thus given by

$$\rho_+(\omega) = Tr(\mu_z D^{(1)}) = P_+(\omega) + V_+(\omega) \quad (18)$$

where

$$P_+(\omega) = \frac{\mu^2}{3KT} b i \omega (c + i\omega) 2L \quad (19)$$

$$b = \beta \hbar^2 / 2I$$

$$c = \left(\frac{1}{\tau}\right) \left(\frac{1}{\hbar}\right)$$

$$\omega_1 = \omega \left(\frac{I}{\hbar}\right)$$

and the equation (18) takes the form

$$\rho_+(\omega) = \mu^2 2L \left\{ \frac{b}{3KT} i\omega_1 (c + i\omega_1) - \frac{i\omega}{2\tau} \Delta_{\ell\ell}^{-1} \langle \ell m | V_{12} | \ell' m' \rangle L \right\} \quad (20)$$

Our main aim is to compute the contribution due to intermolecular interactions in the K-S and G-L models. In the K-S model, the contribution is given by

$$\frac{i\omega}{2\tau} \Delta_{\ell\ell}^{-1} \langle \ell m | V_{12} | \ell' m' \rangle L \quad (21)$$

We know that L is given in (Malo, 1995a) as

$$L = \frac{1}{2b(v + i\omega)^2}$$

In the classical domain where

$$b = \beta \hbar^2 / 2I$$

$$v = 1/\tau$$

Thus the contribution in the classical region will be given by the imaginary part of

$$\frac{i\omega v \langle \ell m | V_{12} | \ell' m' \rangle}{[B + v + i(\omega + \omega_{\ell\ell})](v + i\omega)^2 2b}$$

which after calculations and rearrangements has the following form

$$KS \Rightarrow \frac{v\omega(2AQv^2 - 2bQC) \langle \ell m | V_{12} | \ell' m' \rangle}{(2AQv^2 - 2bQC)^2 + (2AbQ + 2bCv^2)} \quad (22)$$

where

$$A = v + B$$

$$B = \langle \theta \phi | V_{12} | \theta' \phi' \rangle$$

$$C = \omega + \omega_{\ell\ell'}$$

$$Q = 2v\omega - \omega^2$$

In the limit of discrete line structure L has the approximate form

$$L \approx \frac{1}{2} \pi \cot(\pi S) \exp(-bs^2) \quad (23)$$

$$S = ic - \omega$$

$$C = v \left(\frac{I}{h} \right)$$

and we finally obtain the following expression for contribution due to intermolecular forces:

$$KS \Rightarrow \frac{\pi \omega v A V_{12} \exp(-b\omega^2) \sinh(2\pi C)}{4A^2 + C^2 \sinh^2(\pi C) + \sinh^2(\pi \omega)} \quad (24)$$

where $A = v + \beta(\theta\phi)$

$$C = \omega + \omega_{\ell\ell'}$$

(b) Gross – Lebowitz Model

Here no more calculations is warranted since we know from previous works (Malo, 2005; Malo, 1995a) that the contribution for the G–L model will just be a modification of the K–S results in the classical and quantum domains as given by expressions (22) and (24) above. Thus

$$GL \Rightarrow \frac{KS}{I - \pi c \omega \exp(-b\omega^2)}$$

The most important qualitative feature of this theory concerns the frequency ω at which the imaginary part of susceptibility–absorption is a maximum. In the previous works (Malo, 2005; Malo, 1995a) in which the effect of intermolecular interaction was not taken into account, the position of the maximum absorption, as the collision frequency is increased, moves to the lower values of frequency of the impressed field and its amplitude also decreases. In the present communication however, it is shown (Fig. 1) that as we increase the collision frequency, the amplitude of maximum absorption, as is expected decreases but its position is shifted to higher frequencies of the impressed field – Tables 1- 4. Our interpretation of this shift to higher

frequencies of the field is that with intermolecular interaction, one needs stronger impressed fields in order to reorient the molecules in the regions of high collision frequency.

Table 1: $R = 1 \text{ \AA}$

Collision Frequency (ν)	Field Frequency (ω)	Maximum Absorption (G-L x 10^{-3})
2	5	0.13
3	7	0.05
4	9	0.02
5	10	0.01
6	13	0.01

Table 2: $R = 2 \text{ \AA}$

Collision Frequency (ν)	Field Frequency (ω)	Maximum Absorption (G-L x 10^{-3})
2	5	0.76
3	7	0.21
4	9	0.12
5	11	0.07
6	13	0.05
7	15	0.03
8	17	0.02
9	19	0.02
10	21	0.01

Table 3: $R = 3 \text{ \AA}$

Collision Frequency (ν)	Field Frequency (ω)	Maximum Absorption (G-L x 10^{-3})
2	5	8.98
3	7	2.97
4	9	1.41
5	11	0.82
6	13	0.53
7	15	0.38
8	17	0.28
9	19	0.21
10	21	0.17

Table 4: $R = 4 \text{ \AA}$

Collision Frequency (ν)	Field Frequency (ω)	Maximum Absorption ($G-L \times 10^{-3}$)
3	8	153.70
4	9	67.00
5	11	36.26
6	13	22.64
7	15	15.47
8	16	11.23
9	19	8.53
10	20	6.70

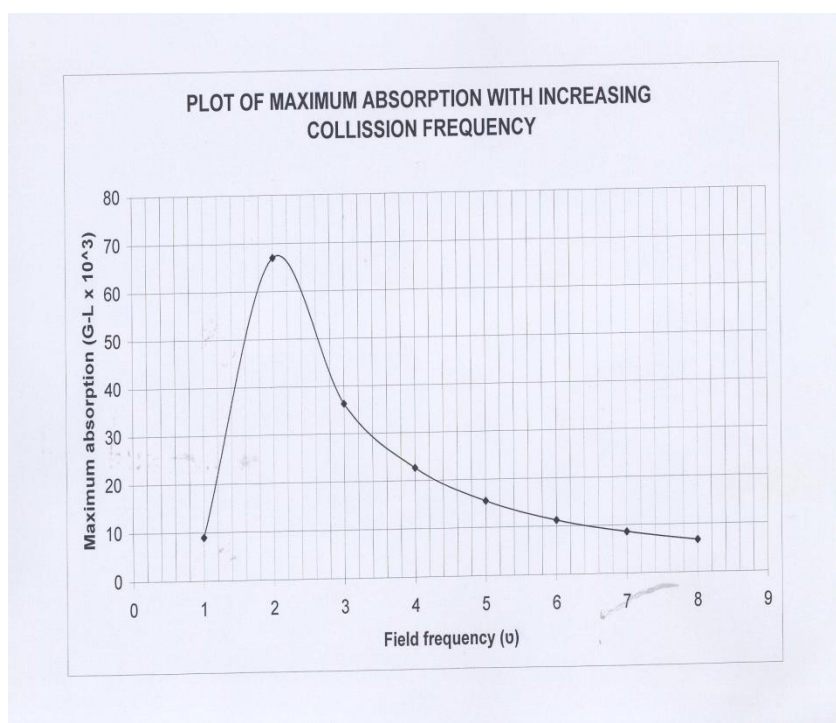


Figure 1. A plot of maximum absorption with increasing collision frequency

CONCLUSION

The present communication is limited to consideration of linear response to an applied field by a linear molecule of moment of inertia I . We have carried out calculations that led to the derivation of integro-differential kinetic equations for both degenerate and non-degenerate internal states. The approximate solution corresponding to the non-degenerate internal states is given in order to obtain the desired effects of intermolecular potential field on the line broadening phenomena. The equations have been derived for both the K-S and G-L collision models. However, the derivations are still based on a single relaxation time characterized by a time τ between collisions.

Needless to mention that this is still a crude model since it implies that there is no variation of line width with rotational quantum number in the quantum domain. In the classical region, it implies that the rotational energy and angular momentum relax at the same rate (Xuan and Mchale, 1998). These integral equations differ from those in our previous works (Malo, 2005; Malo, 1995a) by an additional term of the form

$$\frac{\langle nk | V_{12} | n'k' \rangle}{B(\theta\phi) + \nu + i(\omega_{\ell\ell} - \omega)}$$

for the non-degenerate case, and

$$\frac{\langle nk | V_{12} | nk \rangle}{B(\theta\phi) + \nu + i(\omega\omega_{\ell} - \omega)}$$

for the degenerate internal states. This intermolecular potential can be given a virial expansion and divided into its long range parts (Novikov *et al.*, 2001).

The great success of statistical mechanics is invariably associated with systems in which interaction between particles is either neglected or can be transformed away. Systems under conditions in which interactions play an essential role are vastly more difficult to analyse vigorously and meaningful approximations hard to obtain. Further on we have to be very specific about the system under study in order to choose the relevant corresponding potential model that describes the dynamics of the system. When this is done, say for instance we take the Buckingham potential.

$$V(R) = \frac{\varepsilon}{1 - 6/\alpha'} \exp \left\{ \alpha' \left(1 - \frac{R}{R_m} \right) - \left(\frac{R_m}{R} \right)^6 \right\}$$

For $\alpha' = 13.772$, we will be in a position to plot profiles of the intermolecular interaction contribution to the K-S and G-L models immediately. This is done in the following manner; for a

given ε and R_m , we shall vary the value of R from $R = R_m$ to any desired value of R . For each value of R we shall compute the absorption profile for different values of collision frequencies.

Since the cumulative effect of intermolecular interaction is to increase total polarization, the line widths will appear broadened for specific values of collision frequencies.

Note that Tables 1 - 4 show the dependence of maximum absorption to the collision frequency and the shift to higher frequencies of the impressed field. Buckingham type of intermolecular potential is assumed.

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