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Quantum Chemical Computational Method for the Role of GH and CRH Regulation on Anxiety Symptoms and Response to Treatment

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ABSTRACT

The purpose of this paper is to utilize several classes of bivariate distributions whose conditionals belong to the two and three parameter lognormal distribution, and to some of their extensions. In this paper, the most general bivariate distribution with lognormal conditionals is fully characterized. The new distribution is very general, and contains as a particular case the classical bivariate lognormal distribution. We present quantum chemical computational method based on the conditional specification. In the application part, we have found the values for salivary cortisol of shy and non-shy adults by using the lognormal distribution and the corresponding mathematical figures are obtained in section 3. From these curves, computational results have been analysed and compared with medical conclusion.

1. COMPUTATIONAL METHOD:

This section presents the lognormal distribution and some of its applications. Here, we discuss about the several classes of bivariate distributions whose conditionals belong to the two and three parameter lognormal distribution, and to some of their extensions [9]. The most natural definition of a bivariate lognormal distribution is in terms of the classical bivariate normal distribution. The bivariate lognormal distribution has the probability function:

$$\boldsymbol{f(x,y,\mu,\sum) = \frac{1}{xy|\sum|^{1/2}2\pi} exp\left\{\frac{-1}{2}(z-\mu)^T\sum^{-1}(z-\mu)\right\}, x,y>0} \quad (1.1)$$

Where

$z = (\log x, \log y)^T$, $\mu = (\mu_1,\mu_2)^T$ and $\sum$ is a 2×2 matrix.

(1.1): The lognormal Distribution and Generalizations:

Kmietowick (1984) has used this distribution for modelling the distribution of household and income. An important appealing of family (1.1) is that the marginal and conditional distributions are again lognormal, as in the bivariate normal rate [11].

From the Gibrat (1931) and Kalecki's (1945) original works, the lognormal distribution has been used for modelling data from income and wealth data and as a distribution for firms size, among other applications in economics and business [6,10]. A random variable $\boldsymbol{X}$ has a two-parameter lognormal distribution if its pdf has the form,

$$\boldsymbol{f(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}} exp\left\{\frac{-1}{2}\left(\frac{logx-\mu}{\sigma}\right)^2\right\}, \quad x>0} \quad (1.2)$$

With $\boldsymbol{\mu \in R \quad and \quad \sigma > 0}$. If $\boldsymbol{X}$ has the density (1.2), we write $\boldsymbol{X \sim LN(\mu,\sigma)}$.

Since,

$\log X \sim N(\mu, \sigma^2)$, the pdf in (1.2) admits the representation $X = \exp(\mu + \sigma z)$, where $Z \sim N(0,1)$.

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Since, $\mathbf{\log X\sim N(\mu,\sigma^2)}$, **the pdf in** $\mathbf{(1.2)}$ **admits the representation** $\mathbf{X=\exp(\mu+\sigma z)}$, **where** $\mathbf{Z\sim N(0,1)}$.

When one works with income and wealth data, one is interested in models above a certain threshold parameter $\boldsymbol{\delta}$. Then, if there exists a $\boldsymbol{\delta\in R}$, such that $\boldsymbol{log(X-\delta)\sim N(\mu,\sigma^2)}$, we have a three-parameter lognormal distribution. In this case, the pdf is given by:

$$\boldsymbol{f(x;\delta,\mu,\sigma)=\frac{1}{(x-\delta)\sigma\sqrt{2\pi}}exp\left\{\frac{-1}{2}\left(\frac{log(x-\delta)-\mu}{\sigma}\right)^2\right\},\ x>\delta} \quad (1.3)$$

If $\boldsymbol{X}$ has the pdf (1.3), we write $\boldsymbol{X\sim LN(\delta,\mu,\sigma)}$.

The first extension of (1.2) is a log version of the skew-normal distribution. this distribution will be called log-skew-normal distribution, and has the pdf:

$$\mathbf{f(x;\lambda,\mu,\sigma)=\frac{2}{x\sigma}\varphi\left(\frac{\log x-\mu}{\sigma}\right)\Phi\left(\lambda\frac{\log x-\mu}{\sigma}\right),\ x>0,} \quad (1.4)$$

Where $\boldsymbol{\varphi(z)}$ and $\Phi(z)$ denote the standard normal density and distribution functions and where $\lambda\in\mathbf{R}$ is a parameter which governs the skewness of the density, and $\boldsymbol{\mu\in R}$ and $\boldsymbol{\sigma>0}$.

Obviously, if $\boldsymbol{\lambda>0}$, (1.4) reduces to lognormal distribution (1.2). We will denote the distribution (1.4) as

$$\mathbf{X\ \sim\ LSN(\lambda,\mu,\sigma)}\ [\mathbf{2,3}].$$

The second one is the log version of the classical exponential-power distribution, proposed by Box and Tiao (1973) and widely used in robust Bayesian contexts [4]. The pdf of this distribution is given by:

$$\mathbf{f(x;\beta,\mu,\sigma)=\frac{1}{x\sigma 2^{(3+\beta)/2}\Gamma\left((3+\beta)/2\right)}\exp\left\{-\frac{1}{2}\left|\frac{\log x-\mu}{\sigma}\right|^{2/(1+\beta)}\right\},\ x>0} \quad (1.5)$$

$\boldsymbol{-1<\beta\le 1,\mu\in R}$ **and** $\boldsymbol{\sigma>0}$. When $\boldsymbol{\beta=0}$, we obtain (1.2) [1].

2. APPLICATION:

Stress reactions are by no means universal, and the activation of 'stress hormones', such as glucocorticoids or corticotrophin-releasing hormone (CRH), is not necessarily the mark of a stress response [13]. Some individuals have lower-than-usual release of glucocorticoids in fearful situations, whereas others have higher release [14], and glucocorticoid release has differential effects and antecedents depending on an individual's history and development [5]. The roles of these hormones are nonetheless crucial to our understanding of both resilience and pathology. Glucocorticoid levels have been strongly linked to many pathological conditions [5]. In particular, they have been strongly, and differentially, tied to generalized anxiety and depressive disorders, posttraumatic stress disorder (PTSD) and social anxiety. Each of these areas of research has implicated glucocorticoid levels, either high or low, in the presentation of variable symptoms of anxiety [8]. Although each of these each of these concerns focuses on the presentation of anxiety-like symptoms, the underlying glucocorticoid activities the presenting symptoms are varied. Even high level of glucocorticoid levels is not necessarily problematic, rather this may be an indicator of high energy and activity in some cases [15]. In some, this may reveal that the person is highly engaged in high-energy endeavors, whereas in others, it shows a potentially pathological response to stressors.

Glucocorticoids are responsible for upregulating CRH in the amygdale, frontal cortex, and bed nucleus of the stria terminals [7,16], whereas they downregulate hypothalamic CRH [15]. Levels of circulating CRH can have long-lasting expression independent of concurrent glucocorticoid levels. Both CRH levels and the site of activation, are important to the presentation of anxiety symptoms, such that noting CRH levels alone is also insufficient to understand the response [7]. The purpose of this paper is to explore the interactions of glucocorticoids and CRH in the presentation of anxiety and depressive disorders in an effort to better describe their differing roles in each of these clinical presentations. In addition, we describe ways in which extra-hypothalamic glucocorticoids and CRH, may play important roles in the presentation of clinical disorders. Social anxiety is a biological phenomenon with underlying environmental influences, similar to PTSD or anxiety and depression. We have noticed the three-day average of daily salivary cortisol output from awakening until bedtime in shy and non-shy adults. Although shy and fearful children tend to have high cortisol levels and high reactivity to stress when they are young. In later life, socially anxious individuals may develop a different pattern with reduced glucocorticoid levels and decreased reactivity. As adolescents and adults, these children enter a hypo-arousal phase notable to 'shutting down'. This hypo-arousal arousal phase is marked by decreased energy, decreased reported anxiety, and reduced glucocorticoid levels. Our results indicate that chronic social stress such as that a shy or fearful child might experience, influences the expression of CRH in both the amygdale and the hypothalamic – pituitary – adrenal axis than the non-shy young adults [12].

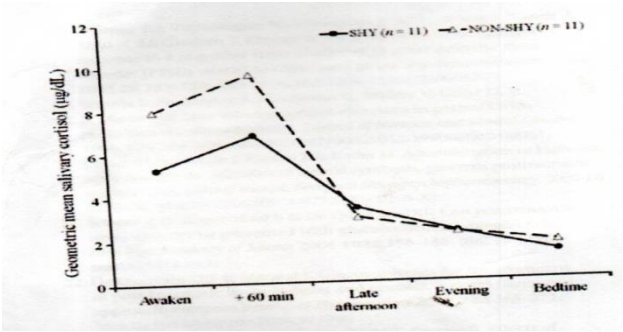

Fig1.Three – day average of daily salivary cortisol output from awakening until bedtime in shy and non-shy young adults.

3. COMPUTATIONAL RESULTS:

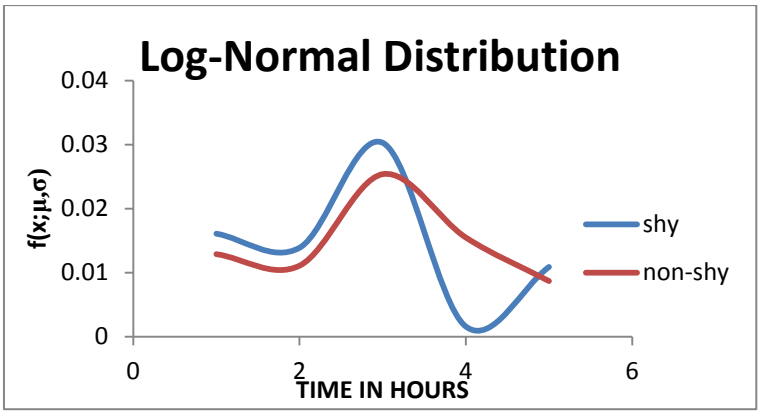

Fig 3.1

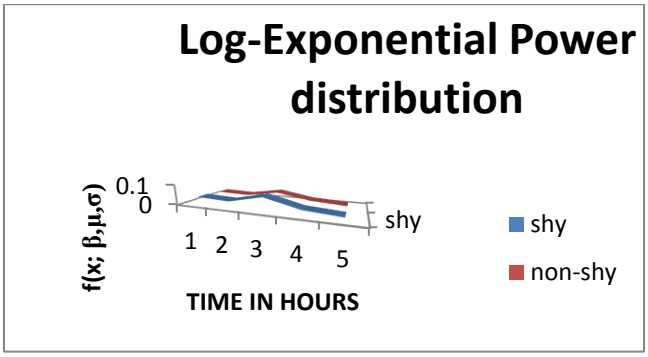

Fig 3.2

4. CONCLUSION:

Glucocorticoids are not just related to stress, but rather to energy levels as well the ability to appropriately regulate these chemicals in a changing environment. In addition, the complex relationship between glucocorticoids and the experience of anxiety indicates that therapy to either reduce or increase glucocorticoid levels is important in the treatment of various conditions including depression/anxiety, PTSD, and social anxiety. Using Log-normal distribution, at the early morning, the salivary cortisol value is 0.0161 for young shy adults whereas for the non-shy adults is 0.0129. After one hour the cortisol vale is 0.0139 for shy adults and 0.0111 in non-shy case. In the afternoon, the value is 0.0303 for young shy adults and for non-shy adults is 0.0254. In the evening time we get 0.0016 for shy and 0.0155 for non-shy adults. During bed-time, the value is low for the two cases, 0.0109 for shy and 0.0087 for non-shy young adults.

Again, we have found the salivary cortisol values by using Log-Exponential power distribution. In this, at early morning, the value for shy adult is 0.0370 and for non-shy is 0.0285. After one hour, the cortisol value for shy people is 0.0301 an for non-shy is 0.0232. In the afternoon, we get the values 0.0662 and 0.0501 correspondingly for shy and non-shy people. In the evening, for shy adults we get 0.0254 and for non-shy adult is 0.0214. During bed-time the value is 0.0129 and for non-shy case is 0.0107.

Even though the difference between the levels of salivary cortisol for shy and non-shy young adults is very small, it gives a considerable attention of GH to both the groups of control and experimental respectively. Glucocorticoids influence mainly the expression of CRH such that high glucocorticoids and high CRH are present in trait fearfulness. The interactions of glucocorticoids and CRH may lead to a reduction in the body's abilities to cope with stressful situations. Although shy and fearful children tend to have high cortisol levels and high reactivity to stress when they are young, in later life, socially anxious individuals may develop a pattern with reduced glucocorticoid levels and decreased reactivity. Also similar to individuals with PTSD, low doses of glucocorticoids administered during exposure for social anxiety have been shown to decrease the anxiety response.

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