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Double-Exponential-X Family of Distributions: Properties and Applications

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Abstract

A new family of distribution named Double-Exponential-X family is proposed. The proposed family is generated from the double exponential distribution. The forms of the probability densities and hazard functions of two distinct subfamilies of the proposed family are examined and reported. General properties such as moment, survival, order statistics, probability weighted moments and quartile functions of the models are investigated. A sub family of the developed family of double –Exponential-X family of the distribution known as double-Exponential-Pareto distribution was used to fit a real life data on the use of antiretroviral drugs. Montecarlo simulation of Efficacy of antiretroviral drugs is conducted to evaluate the performance of the model. The models were tested using some models diagnostic tests and it was revealed that the proposed model was better than the ones proposed before it from the same family and also, the stochastic dominance method was used to affirm the best antiretroviral drugs used in the study.

Keywords: Double Exponential Distribution, Hazard Function, Molecular Simulation, Stochastic Dominance.

1. Introduction

In the past few decades, a variety of classical or general distributions have been widely used to structure data in the fields of engineering, actuarial, environmental science, biology, demography, economy, insurance, and finance. Despite this, there continue to be problems in each of the aforementioned fields. Naturally, this may be attributed to the fact that, as a result of the growth of science and technology, the underlying distributions are no longer able to suit the data set. Because of this, it is necessary to create new kinds of extended distributions that can handle these fresh difficulties. As a result, numerous methods have been proposed and researched to develop or introduce new families of distribution by including a parameter or several parameters in the baseline random variable model while providing a great degree of flexibility in actual data modeling, including beta-G [1,2], Gamma-G type-1 [3], Mc-G [4], Log-Gamma-G Type-2 [5], Gamma-G type-3 [6], Weibull-X family of distributions [7], odd generalized exponential-G [8,9], type-1 half-logistic family [10], Kumaraswamy-Weibull-generated family [11], new Weibull- G family [12], generalized transmuted- G [13]

Taking $v(t)$ to be the probability density function (PDF) of a random variable, say, which belongs to m and n, that is T$\in [m,n]$ for -$\infty \leq$ m < n <∞ and also, let $W[F(x,\xi)]$ be a function of cumulative distribution function (CDF) of a random variable, say X which depends on the parameter ξ which satisfies the conditions:

i $W[F(x,\xi)]$ is bounded between m and n

ii. $W[F(x,\xi)]$ is differentiable and monotonically increasing

iii. $W[F(x,\xi)] \rightarrow$m as x$\rightarrow$-∞ and $W[F(x,\xi)]\rightarrow$n as x$\rightarrow\infty$

The CDF of the T-X family of distribution as recently used by [14] as

$$G(x) = \int_{m}^{w(F(x;\xi))} v(t)dt \ , \qquad x \in R \qquad (1)$$

And the PDF corresponding to (1) is given as: $g(x) = \left\{\frac{d}{dx} w[F(x;\xi)]\right\} V\{w[F(x:\xi)]\} \qquad x \in R$

Several new families of distributions have been postulated using the concept of T-X family as proposed [14]. Different functions of $W[F(X;\in)]$ have been employed in the literature for the T-X family which are revealed in Table1.

This research aims to introduce a new family of continuous distributions, which is named as Double Exponential-X ("DE-X" for short) family. This family's two distinct sub-models are looked into and discussed. Both real life and simulated data are used to illustrate the essence of the new model in the area of applied science.

This paper's remaining sections are divided as follows: In the section titled "Double-Exponential X family," we define the DE-X family of distributions, provide a mathematical derivation of some of the family's fundamental statistical properties, including the moment, survival function, order statistics, probability weighted moment (PWM), and quartile function, and provide a maximum likelihood estimation method for determining the model parameters. The DE-Pareto Distribution sub-model constructed from this family was fitted to real- life data of viral load (Copies/ml) of some patients receiving antiretroviral medication. In order to calculate the average binding affinity

of Abacavir and Neviranpine as they docked (using molecular docking), simulated data (from simulation of molecular dynamics) was also used.

Table 1: A few T-X Family Members Currently in Existence

$W[F(x;\xi)]$	Range of X	Members of T – X family
$F(x,\xi)$	(0,1)	Beta – G [1]
$-\log[F(x;\xi)]$	$(0,\infty)$	Gamma-GType-22) [15]
$-\log[1-F(x;\xi)]$	$(0,\infty)$	Gamma-GType-1[3]
$\frac{F(x,\xi)}{1-F(x,\xi)}$	$(0,\infty)$	Gamma-GType-3 [6]
$-\log[1-F(x,\xi)]$	$(0,\infty)$	Exponentiated T – X [14]
$\log\left\{\frac{F(x,\xi)}{1-F(x,\xi)}\right\}$	$(-\infty,\infty)$	Logistics – G [16]
$\log[-\log\{1-F(x,\xi)\}]$	$(0,\infty)$	The logistic – X family [8,9]

2. Materials and Methods

2.0 The Double Exponential-X Family

Given the PDF of the double exponential distribution

$V(x;b;\mu)=\frac{1}{2b}e^{\frac{|x-\mu|}{b}}$ (21) (2)

And the corresponding CDF with high reliability on the support is given by:

$F(x;\mu;b)=\frac{1}{2}e^{\frac{-(\mu-x)}{b}}$ if$x\leq\mu$ (3)

$F(x;\mu;b)=1-\frac{1}{2}e^{\frac{-(x-\mu)}{b}}$ if$x\geq\mu$ (4)

Then, if $x\geq 0$, then the CDF changes to

$F(x;b)=1-\frac{1}{2}e^{-\frac{x}{b}}$ (5)

And its corresponding PDF is given as:

$V(x;b)=\frac{1}{2b}e^{\frac{-x}{b}}$ (6)

If x follows (6) and setting $W[F(x,\xi)]=\frac{1}{1-F(x,\xi)}$ in (1), we define the CDF of the Double Exponential-X family by

$G(x,b,\xi)=\frac{1}{2}[1-e^{-\frac{1}{b}(W[F(x,\xi)])}]=\frac{1}{2}-\frac{1}{2}e^{-\frac{1}{b}(W[F(x,\xi)])}$, $b,\xi>0$, $x\in R$ (7)

Where the baseline distribution's CDF, which is dependent on the vector parameter, is denoted by $F(x,\xi)$,

ξ and $W[F(x,\xi)]=\frac{1}{1-F(x,\xi)}$ is a special transformation. The corresponding PDF is obtained via the first derivative of the CDF, $G(x,b,\xi)$ and it is shown by:

$$g(x,b,\xi)=\frac{1}{2b}\left[\frac{d}{dx}(W[F(x,\xi)])\right]e^{-\left\{\frac{1}{b}(W[F(x,\xi)])\right\}},\quad b,\xi>0 \qquad (8)$$

$g(x,b,\xi)=g(x,b,\xi)=\frac{1}{2b}[(W[F(x,\xi)])']e^{-\left\{\frac{1}{b}(W[F(x,\xi)])\right\}}$, where $(W[F(x,\xi)])'=\frac{d}{dx}(W[F(x,\xi)])$ and $b,\xi>0$

The motivations behind using DE-X family in the real life situations include:

- It is a popular technique for inserting extra parameter(s) to produce an expanded baseline distribution,
- To enhance the properties of the traditional distributions,
- To continuously offer better fits compared to other produced distributions with the same or more parameters,

2.1 Special Sub-Models

Most often for one reason or another, extended versions of distributions are introduced for the following reasons;

1. An alternate model to the existing distribution that has been successfully applied in the past
2. A flexible statistical model that provides a good match to the data
3. A model with closed CDF, Survival Function (SF), Hazard Rate Function(HRF) forms and a strong propensity to lessen estimation challenges.

Thus, we introduce two unique sub-models of the DE-X family that have at least one of the aforementioned characteristics.

2.1.1 The DE-Pareto (DE-P) distribution

The PDF and the CDF of the Pareto random variable are

$f(x, \theta, \alpha) = \frac{\alpha(\alpha^{\theta})}{x^{\theta+1}}$ and $F(x, \alpha, \theta) = 1 - \left(\frac{\alpha}{x}\right)^{\theta}$, x>0, α, θ>0, .

Then the CDF and the PDF of the DE-P model are given by (9) and (11) respectively.

$$G(x, b, \alpha, \theta) = \frac{1}{2} - \frac{1}{2} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}, \text{ b}, \theta, \alpha > 0 \quad (9)$$

Hence, $$G(x, b, \alpha, \theta) = \frac{1}{2}(1 - e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}) \text{b}, \theta, \alpha > 0 \quad (10)$$

Hence, $$g(x, b, \alpha, \theta) = \frac{\theta}{2\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}, x, \text{ b}, \theta, \alpha > 0 \quad (11)$$

Plots of the DE-P density and Hazard rate function for selected parameter values are presented in Fig.1 and Fig.2 respectively below:

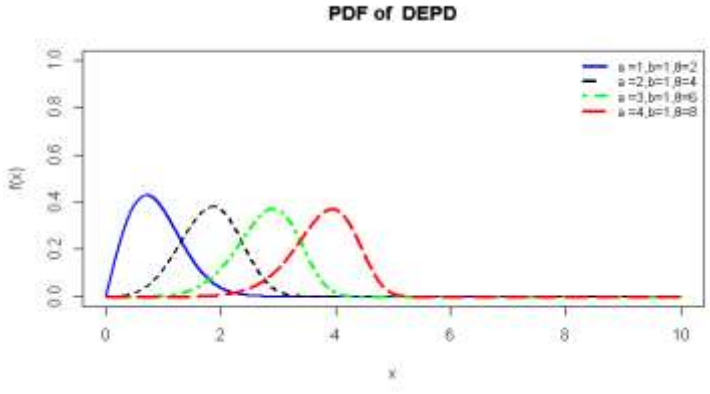


Figure.1:PDF plot at fixed b =1 and increasing α *and* θ

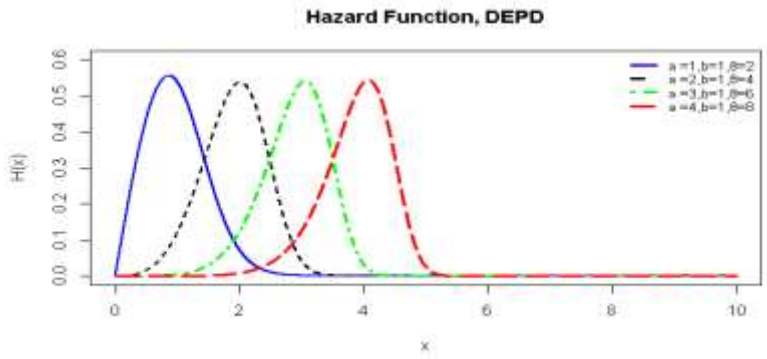


Figure.2: Hazard plot at fixed b =1 and increasing α *and* θ

2.1.2 The DE-ParetoII (DE-P2)

Given the PDF and CDF of the Pareto type-2 distribution$f(x,a,b) = \frac{b}{a}\left(\frac{a}{x-a}\right)^{b+1}$, b,a, $x > 0$ and $F(x;a,b) = 1 - \left(\frac{a}{x-a}\right)^{b}$, x, b,a,$> 0$.

Then the CDF and PDF of DE-PII model are given as

$$G(x,b,a,\xi) = \frac{1}{2}\left[1 - e^{-\frac{1}{b}\left(\frac{x-a}{a}\right)^{\theta}}\right], \text{a,b,}\theta > 0;\ x > 0\ 0 \qquad (12)$$

For the PDF,

$$g(x,\text{a},\text{b},\xi) = \frac{\theta}{2ba}\left(\frac{x-a}{a}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x-a}{a}\right)^{\theta}}, \text{ a, b, } \theta > 0\ ;x > 0 \qquad (13)$$

Fig.3 and Fig.4 give the plots of the PDF and HRF of DE-PII distribution for selected parameter values.

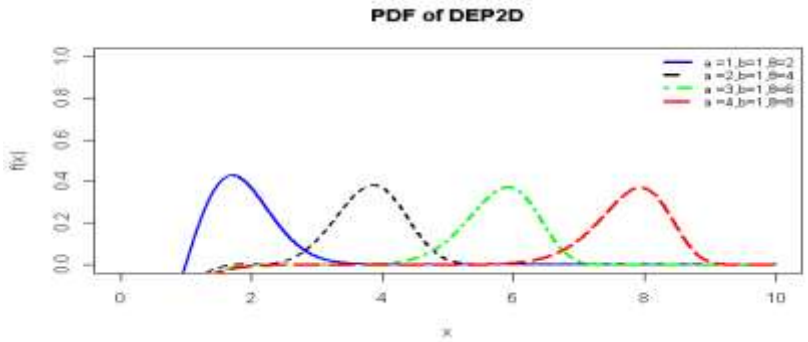


Figure.3 The pdf of double exponential-ParetoII distribution at different values of parameters

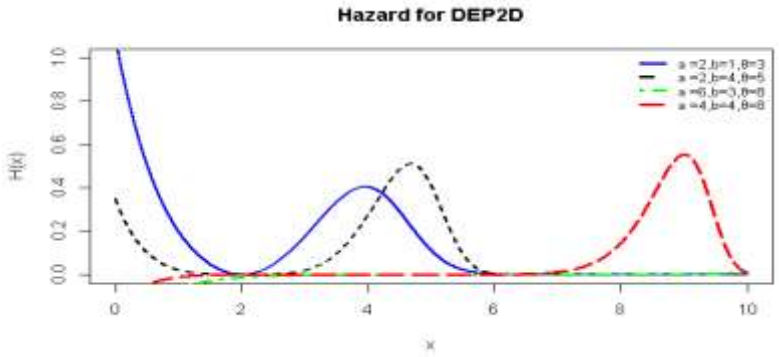


Figure.4 showing the hazard of double exponential-ParetoII distribution at different values of parameters

2.2 Basic Mathematical Properties of DE-Pareto

Here, we provide the basic properties of DE-X family of distributions.

2.2.1 Moments of DE-Pareto

Assuming X follows DE-X family with density $g(x, \mathrm{a}, \mathrm{b}, \xi)$, then its r^{th} moment is

$\mu_r{}^1 = \int_{-\infty}^{\infty} x^r \; g(x, a, b, \xi) d_x$

$$E(X^r) = \int_0^{\infty} x^r \frac{\theta}{2\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}} dx \quad (14)$$

$$E(X^r) = \frac{1}{2}\left(\alpha \sqrt[\theta]{b}\right)^r \Gamma\left(\frac{r}{\theta}+1\right)$$

$$E(X) = \frac{\alpha \sqrt[\theta]{b}}{2} \Gamma\left(\frac{1}{\theta}+1\right); \; r=1 \quad (15)$$

Variance:

$$Var(X) = \left(\alpha \sqrt[\theta]{b}\right)^2 \left[\frac{1}{2}\Gamma\left(\frac{2}{\theta}+1\right) - \left(\frac{1}{2}\Gamma\left(\frac{1}{\theta}+1\right)\right)^2\right] \quad (16)$$

2.2.2 Survival Function of DE-Pareto

The survival function of DE-X family is given as

$$S(x) = 1 - G(x, b, \alpha, \theta) \quad (17)$$

$$S(x) = \frac{1}{2}\left(1 + e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}\right) \quad (18)$$

2.2.3 Probability Weighted Moments of DE-Pareto

The Probability Weighted Moment (PWM) of DE-X random variable is

$$M_{rs}(x) = \int_{-\infty}^{\infty} x^s \, g(x, b, a, \xi) G(x, b, a, \xi))^s d_x \quad (19)$$

2.2.4 Hazard Function of DE-Pareto

$$H(x; \alpha, b, \theta) = \frac{g(x)}{S(x)} = \frac{\frac{\theta}{2\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}}{\frac{1}{2}\left(1+e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}\right)} = \frac{\frac{\theta}{\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}}{1+e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}} \quad (20)$$

2.2.5 Renyi Entropy of DE-Pareto

$$\delta_r = \frac{1}{1-r} log \int_0^{\infty} f^r(x) dx = \frac{1}{1-r} log \int_{\mathbf{0}}^{\infty} \left(\frac{\theta}{2\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}}\right)^{\boldsymbol{r}} dx \quad (21)$$

$$\delta_r = \frac{1}{1-r}\, log\, \left(\frac{b\theta}{2r\alpha b}\sqrt[\theta]{\frac{r}{b}}\right)^r \left(\frac{\alpha}{\theta}\sqrt[\theta]{\frac{b}{r}}\right) \Gamma\left(r - \frac{r}{\theta} + \frac{1}{\theta}\right) \quad (22)$$

2.3. Estimation

We describe the maximum likelihood method of estimation in this section for the unknown parameters of the DE-X family. The method of Maximum Likelihood estimation is adjudged to be the best method of estimating parameters of distributions.

2.3.1 Maximum Likelihood Estimation DE-Pareto

In this, let $X_1, X_2, \dots, X_k$ be the observed values for DE-X distribution with parametersb, a, ξ. The total log-likelihood function corresponding to (11) is presented as Log

$$\mathrm{L}(x, b, a, \xi) = \prod_{i=1}^{n} \frac{\theta}{2\alpha b}\left(\frac{x}{\alpha}\right)^{\theta-1} e^{-\frac{1}{b}\left(\frac{x}{\alpha}\right)^{\theta}} \quad (23)$$

3. Results

3.1 Fitting the Model to Molecular Dynamics Simulated Data

The two approved HIV drugs were obtained from The Drug bank archive online, modeled using (Spartan'14 version 1.18 by wave function Inc)

i. Geometry optimization and calculation of the two drugs were done using density functional theory (DFT) with 6-31G* basis set to obtain the molecular parameters responsible for the cytotoxicity of the compounds under investigation and then saved as pdb files for simulation study

ii. The protein receptors responsible for HIV(that is, the HIV-causing organisms) used were gotten from protein data bank (PDB) [18]

iii. with no missing residues and a single strand were obtained by deleting multiple ligands, non-protein and other protein parts from the pdb files. Autoduck tools version 1.5.6 was used to locate the binding site and to add hydrogen to the prepared protein receptor and finally converted to a protein data bank format (pdbqt) for the molecular simulation. Autodockvina were used for the simulation process and the simulation was repeated for seven different in order to obtain the most stable conformation of the drug-receptor complex and post docking analysis was done using EduPymolversion 1.7.4.4 and discovery studio 4.1 visualizer.

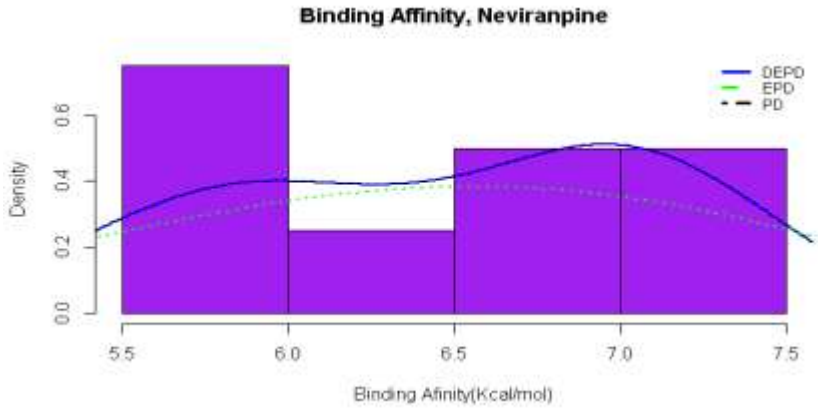


Figure 5a: Fitting the Models to Neviranpine data (Obtained via Molecular Simulation)

From the figure 5a above, we can say that the selected distributions approximately follow the distribution of the data, thus, making the distributions suitable for data collected when using Neviranpine to dock HIV protein receptor

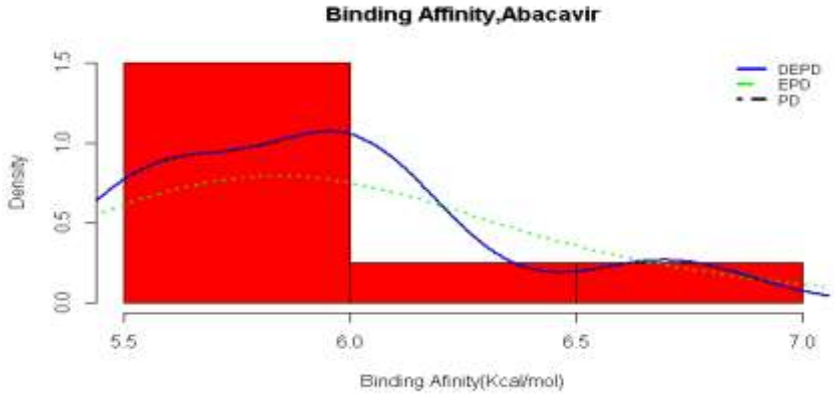


Figure 5b: Fitting the Models to Abacavir data (Obtained via Molecular Simulation)
From the Fig. 5b above, we can say that the selected distributions approximately follow the distribution of the data, thus, making the distributions suitable for data collected when using Abacavir to dock HIV protein receptor

Table1. Fitting cells table with the including numbers

Model	Parameter	Criteria	Mean Affinity
EPD	$\hat{\theta}$ $= 0.029978(0.034)$ $\hat{\alpha} = 0.9980(0.367)$ $\hat{b} = 0.996486(0.648)$	AIC=303.405 BIC=303.6433 CAIC=309.405	1.663157(0.902308)
DEPD	$\hat{\lambda}$=1.978e+06(1.639e-02) $\hat{\theta} =$ 1.503e-04(5.307e-05) $\hat{\beta}$=9.024e-01(2.211e-04)	AIC =-27203950 BIC= -27203950 CAIC=27203944	0.4511979(0.225)
PD	$\hat{\alpha}$= 8.089e+03 (7.567e-02) $\hat{\beta}$ =(3.372e+03) 9.268e-02	AIC=-810083 BIC=-810082.8 CAIC=-810080.6	3.3724(0.41697)

From table 2 above, we can say that the parameter of the model is stable and the Double exponential Pareto distribution (DEPD) appears to be the best of all the competing model (model with the lowest information criteria is the best of all the models). The 45.1198% of the binding affinity is attributed to Neviranpine.

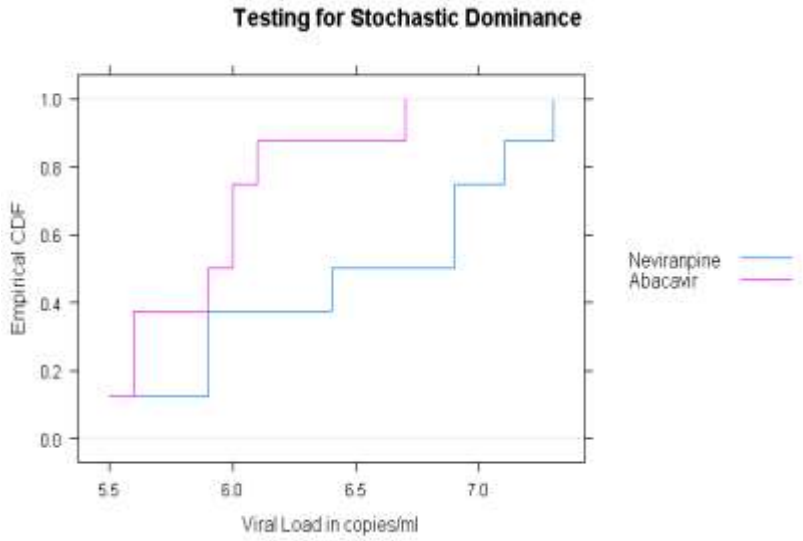
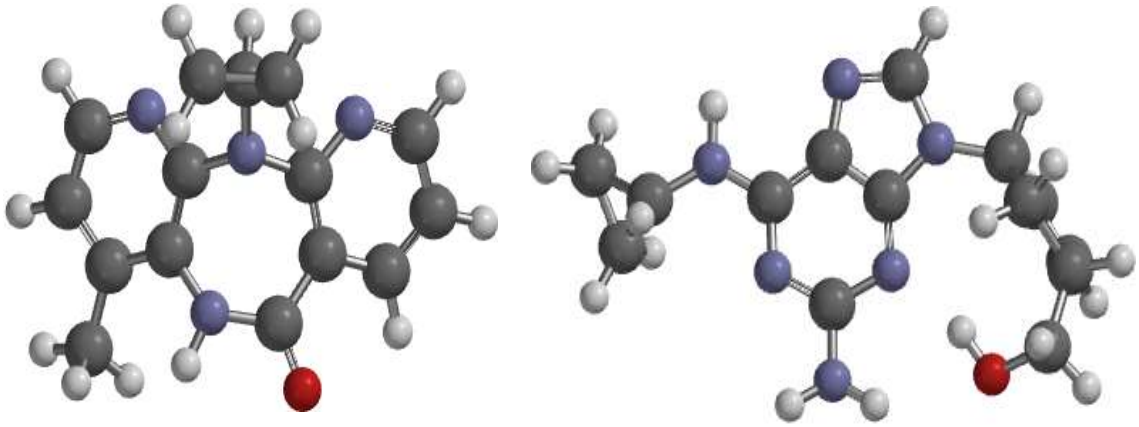


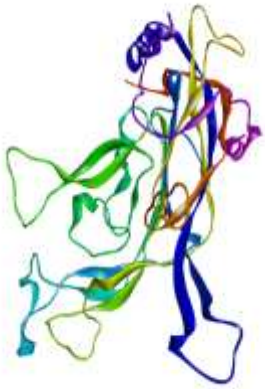
Fig 4: Investigating Stochastic Dominance

From fig 4 above, we can say that Neviranpine is first order (Stochastically) dominated Abacavir. That is, the mean effect of Nevirapine has dominated that of Abacavir when it comes to the viral load measurement (copies/ml) from the patients subjected to Anti-retroviral therapy.

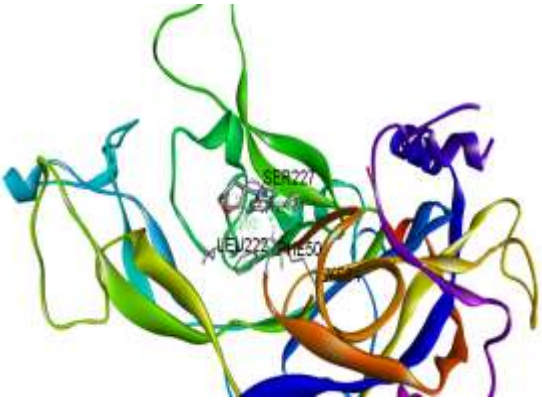


3D Structures of Nevirapine **3D of Abacavir**

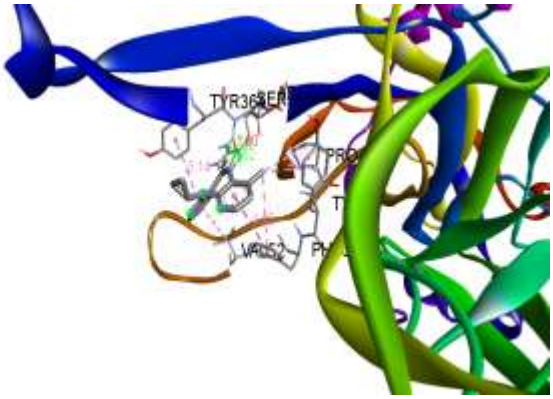
Figure 5: The Ligands (Nevirapine and Abacavir) used as the drug in Anti-retroveral therapy



3D Receptor Responsible for HIV (Protein responsible for HIV)



Interaction of Abacavir and 3PLT



Interaction of Nevirapine and 3LPT

Figure 6. The Docking Result of Abacavir and Nevirapine

The Abacavir and Nevirapine were used as the Ligands to dock HIV protein receptor, the fig 6 showed interaction between the ligands and HIV protein receptor.

Table 5: The Molecular Properties of the Drug used in this study (Molecular Docking)

Molecular Formula	$C_{15}H_{14}N_4O$	$C_{14}H_{18}N_6O$
Molecular Weight	266.30amu	286.34amu
Area	$281.25A^2$	$305.46A^2$
Volume	$269.04A^3$	$285.66A^3$
Polarizability	62.14	63.34
Hydrogen Bond Donor (HBD)	1	2
Hydrogen Bond Acceptor (HBA)	5	5
Polar Surface Area (PSA)	36.84	67.47
Ovality	1.40	1.46
Log P	0.13	0.16
Dipole Movement	2.33	1.93D
HOMO	-5.80Ev	-5.28eV
LUMO	-1.32eV	-0.16eV
BG	4.58eV	5.12eV

4. Discussion

From Table5, the properties of the drugs used in determining the toxicity are clearly displayed, as behavior, and the general effect of each drug on the body system. Parameters such as HBA, HBD, PSA, LogP and polarizability are used to determine if a particular compound is a good drug candidate. This reveals the active properties of the drugs used in determining the cytotoxicity of each drug towards the receptor responsible for HIV. Failure of most drugs in clinical experiments is a result of there poor ADME (Absorption, Distribution, Metabolism and Excretion) properties, hence for a ligand to be chosen as a drug candidate with good ADME properties HBD must be less than five, HBA must be less than ten and its molecular weight in g/mol must be below 500, any ligand that violates this set of rules might result to the problem if ingested [19].

Polar Surface Area (PSA) gives information about the ability of a drug-like compound to penetrate into the cell membrane. It has been established that ligands with high PSA value greater than $140Å^2$ will have poor penetrating power into the cell membrane. On the other hand, molecules with PSA value below $60Å^2$ will have high penetrating power [20]. Hence, we are expecting high penetrating power into the cell membrane from Abacavir and Nevirapine, and these are used to determine if a particular compound is good drug candidate.

The docking result used for stochastic dominance in order to determine the most effective drugs that perform actively in curing the diseases shows better binding affinity and inhibition constant from Nevirapine as compared to Abacavir and this is an indication that Nevirapine drug is more potent for curing the disease(HIV).

5. Conclusion

A new family of distribution (Double Exponential-X family) has been introduced. Two distinct sub-models of the distribution were discussed. It is shown that the two special models' densities can generally be skewed to the left or right, symmetrical, reverse j-shaped, and can also have both growing and decreasing, as well as, of course, unimodal. The maximum likelihood estimation approach is used to estimate the parameters. A molecular simulation study that compares the newly

built model's performance to previous well-known distributions is presented. There are derived and explained several fundamental mathematical characteristics of the new family. Finally, real-life applications of the model to data sets on the effectiveness of various antiretroviral medications were provided, and they compare favorably to other well-known distributions in terms of data fit, and the efficacy of the pharmaceuticals utilized was compared using the stochastic dominance approach.

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