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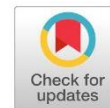
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Phytochemical Screening and Antibacterial Activity of *Moringaoleifera* Leaf Extract Western Libya

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Abstract

Moringa oleifera (M. oleifera) is one of the Moringaceae family. M. oleifera plant parts retain a precious pharmacological effect. Its leaves are utilized commonly because of having enormous nutrients as nutraceuticals. Moreover, its compresses various effects such as biological and antimicrobial effect as antibacterial or antifungal. Additionally, M. oleifera investigationin was carried out either in vivo or in vitro to conclude that their leaves component has pharmacological effect. This current study had confirmed therapeutic effect of *Moringa Oleifera* leaf extract and its antibacterial activity. There is critical need for more advanced research about use and pharmaceutical effects of *Moringa Oleifera* leaves in improvement of various drugs and useful foods. This study aimed to investigate phytochemical ingredients and antibacterial effect of *Moringa Oleifera* leaf extract and the uses of *Moringa Oleifera* leaf extract either traditionally or pharmacologically concluded.

Keywords: *Moringaoleifera*, Antibacterial activity, Phytochemical screening, Libya.

INTRODUCTION

The drumstick tree, or *Moringaoleifera* Lam., is a member of the Moringaceae family and is extensively dispersed in various regions, including tropical and desert nations, as well as in India and Africa. It was primarily used for food and medicine (Al_husnan & Alkahtani, 2016). *Moringaoleifera* has numerous qualities that may be used for food, medicine, and other industrial and home applications (Falowo et al., 2018; Padayachee & Baijnath, 2020), particularly its leaves, which may be eaten raw, roasted, or dried and kept for a long time without losing any of their nutritional value. In addition to using the leaves for food and feed, they may also be used as functional foods or nutraceuticals since they naturally contain phytochemicals such as flavonoids, carotenoids, and glucosinolates (Amaglo et al., 2010; Sultana et al., 2009). The main phytochemicals found in moringa leaves are astragalin, isoquercetin, and crypto-chlorogenic acid, which have anti-oxidant, anti-hypertension, and anti-inflammation characteristics (Verma et al., 2009; Vongsak et al., 2012).

Based on the bioactive components and their antioxidant activity, several in vitro experiments have largely supported the biological activity of these plant extracts (Leone et al., 2015; Sultana et al., 2009). Its strong antioxidant properties are principally brought on by its high phenolic content. Due to these therapeutic advantages, several pharmaceutical preparations from this plant have been manufactured and sold in both the Indian and global markets.(Mehra et al., 2020; Sahakitpichan et al., 2011) Different sections of *M. oleifera* have antibacterial potentials that can be used to purify



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water, eliminate biofilm threats, and eradicate pathogenic microbes. The long-term use of *M. oleifera* and its ethno-pharmacological characteristics have proven its safety. *M. oleifera* has also been employed for bio-enhancement and as nanoparticles in medication administration in addition to its antibacterial action (Arora et al., 2013). Fidrianny et al. study mentioned that *M. oleifera* is commonly named Sanjana and drumstick. The name Moringa originated from murungai; a Tamil word that means twisted pod (Dhakad et al., 2019; Fidrianny et al., 2021) study illustrated that the cultivation of Moringa has different reasons according to its nutritional content or medicinal uses (Djemoui et al., 2019). *M. oleifera* has medicinal effects documented by (Djemoui et al., 2019). study, such as hypoglycemic effect, antioxidant, antibacterial, antifungal, and wound healing due to anti-inflammatory activity (Djemoui et al., 2019). (Amaglo et al., 2010) reported that the leaves, in particular, can be used in a salad, roasted, or kept as dry powder for a prolonged time without losing nutritive constituents (Amaglo et al., 2010).

Moringa leaves were reported by (Maheshwari et al., 2014). to have elevated amounts of protein that could be utilized as food. Also, they mentioned that *Moringa oleifera* contains a high amount of provitamin A. (Tshabalala et al., 2020). traced the source of the cardiovascular benefit and body energizing to the omega-3 and omega-6 polyunsaturated fatty acid content of Moringa. It can be used for obese patients due to low calorific value (Kashyap et al., 2022; Maheshwari et al., 2014)

They also illustrated calcium contents and digestible protein that is higher than milk. (Kasolo et al., 2010). mentioned moringa leaves' high content of potassium, magnesium, and copper. Iron content is 28 times of spinach, proved (Fuglie, 1999; Kasolo et al., 2010). Interestingly, Mbikay approved that fat-soluble vitamins like D and E and water-soluble like folic acid, nicotinic acid, and vitamin care also exist in *M. oleifera* (Mbikay, 2012). Stevens et al. mentioned that leaves are not toxic when taken in large amounts, so it is found to be safer and healthier for consumption (Stevens et al., 2013). Bacterial species develop drug resistance to common antibacterial agents. So, medicinal plants such as Moringa leaves could be used as alternative treatments for infectious diseases (Luqman et al., 2012).

Rios & Recio's studies reported the need for more studies on the antibacterial activity of essential oils or compounds like alkaloids, flavonoids, diterpenes, and triterpenes to justify the use of medicinal plants (Rios & Recio, 2005), while Abdallah mentioned that metabolites of *Moringa oleifera* leaves, such as alkaloids, flavonoids, and saponins have wonderful pharmacological effects as antibacterial and anti-microbial properties and interestingly as anticancer on (Berkovich et al., 2013). study (Abdallah, 2011; Berkovich et al., 2013).

MATERIALS AND METHODS

Collection and Identification of Plant Material

Moringaoleifera tree leaves were collected. The leaves were washed under distilled water for dust and foreign particle removal. After that, the leaves were air-dried in an oven at 60°C. The dried leaves were added to a mixer to be ground into fine powder. The fine powder was stored in a refrigerator to avoid heat and light exposure and kept for further use.

Preparation of Plant Material

About 10g of the fine powdered *Moringaoleifera* leaves were suspended in 100 mL of ethanol and shaken well. The suspensions were kept at room temperature for 24 hours. The suspensions were then filtered. The solvent was removed by heat treatment at 80 °C to concentrate the extract. The extracts were stored in a refrigerator at 4°C for further analysis (Abadallah & Ali, 2019).

Phytochemical Screening

The collected plant extracts were subjected to qualitative phytochemical analysis for identification of various bioactive chemical constituents (alkaloids, volatile oils, saponins, flavonoids, steroids, tannins, and terpenoids) conducted using standard laboratory methods as described by (Edeoga et al., 2006; Sofowora, 1993).

Test Isolates

Clinical *Staphylococcus aureus*, *Streptococcus pyogenes*, and *Pseudomonas aeruginosa* isolates were collected for testing the antibacterial activity of *Moringaoleifera*. As described by Cheesbrough, gram staining and microbiological analysis were used in recognizing the isolates by utilizing differential media and biochemical tests.

Antibacterial activity testing

0.1 ml of each organism culture was inoculated onto the plates' surface by a sterile swab stick. The plates were incubated for 24 hours at 37°C, after which the inhibition zones were calculated using a meter ruler.

All the experiments were repeated three times, and the mean was recorded.

RESULTS

Phytochemical Screen

1. Tannins: A green color and gelatinous precipitate resulted upon adding 1 ml of 1% Lead acetate to 1 ml of the moringa leaf extract in a test tube. This result confirmed the existence of tannins.
 2. Saponins: Durable white precipitate resulted when 1-3 ml of mercury chloride was added to 5 ml of leaf extract which was judged as an indicator of saponins existence.
 3. Flavonoids: A yellow shade that signified flavonoids resulted when moringa leaf extract was added to diluted ammonia and concentrated sulphuric acid.
 4. Terpenoids (Salkowskitest): No brown color resulted when 1 ml of leaf extract was added to chloroform, one drop of concentrated sulphuric acid, and one drop of anhydrous acetic acid.
 5. Resins: Turbidity resulted when the leaf extract was added to the ethyl alcohol (95%) solution
 6. Volatile oils: A shiny pink layer on filter paper formed after UV light exposure after the filtration of leaf extract, indicating volatile oils' content.
 7. Alkaloids: A grey color confirmed alkaloids' presence when adding leaf extract to 2 ml of Marquis Reagents.
 8. Glycosides: A few drops of Fehling reagent were added to 1 ml of leaf extract.
- (Table 1) lists the phytochemical components of moringa leaf extracts.

Table: (1). Illustrate the phytochemical constituent of moringa leaf extract.

Phytochemical constitutes	Result
Alkaloids	++
Saponins	+
Tannins	+++
Flavonoids	+
Terpenoids	-
Resins	+++
Volatile oils	+++
Glycosides	++

Symbol: +=Existence of phytochemical, -=Absence of phytochemical. (+++)high, (++) medium, (+) poor, (-)no found

The results indicate the presence of saponins, resins, tannins, alkaloids, flavonoids, glycosides and volatile oils, and the absence of terpenoids.

Antibacterial Activity:

The antibacterial activity of *Moringa Oleifera* leaf extract is summarized in (Table 2).

The inhibition zones emphasized that it depends on the type of bacteria and concentration of *Moringa Oleifera* leaf extract. The highest zone of inhibition is demonstrated by *Pseudomonas aeruginosa* (17 mm) in concentrated extract and (14mm) in diluted extract.

Interestingly, the case of *Staphylococcus aureus* and *Streptococcus pyogenes* reported zero results which indicates their negative results and the antibacterial activity of *Moringa Oleifera* leaf extract.

Table: (2). Demonstrate the antibacterial activity of *MoringaOleifera* leaves extract

Name		Result
Staphylococcusaureus	Concentrated	0
	Diluted	0
Streptococcus pyogenes	Concentrated	0
	Diluted	0
Pseudomonasaeruginosa	Concentrated	17
	Diluted	14

DISCUSSION

Chhetri *et al.* study reported that bioactive constituents can be taken from plant parts like seeds, roots, stems, leaves, and flowers (Chhetri et al., 2008). The results of our study showed the existence of bioactive components in moringa leaf extracts. Our study revealed the presence of alkaloids, volatile oils, saponins, resins, etc., in the ethanol extract of the leaves as in (Table1). The outcome of the current study is in a parallel line with previous studies that screened the phytochemical composition of moringa leaves. Moringa leaves were proven to include numerous phytochemicals (Edeoga et al., 2006; Madziga et al., 2010).

The phytochemicals have remarkable pharmaceutical effects that are used in drugs for treating sclerosis, diabetes, skin antiseptic, diarrhea, colitis, and cancer.(Aboaba et al., 2011; Madziga et al., 2010). studies illustrated that Alkaloids, for example, are extensively used as anticancer agents, aesthetics, and central nervous stimulants. Alkaloids also have metabolic effects and control development in living systems (Aboaba et al., 2011; Madziga et al., 2010).(Mir et al., 2013). mentioned the role of saponins as one of the phytochemicals in cholesterol lowering. Tannins containing plants are commonly used as mouthwashes, and eye washes, as mentioned by (Abadallah & Ali, 2019; Mir et al., 2013).

They also mentioned that terpenoids are effective as antimicrobial, anti-inflammatory, and immunomodulatory agents and in the case of cancer. (Abadallah & Ali, 2019) explained the result of moringa leaf extracts' antibacterial activity achieved in our study against the clinical isolates of *Staphylococcus aureus*, *Streptococcus pyogenes*, and *pseudomonas* (Abadallah & Ali, 2019).

The outcome of our study was in line with (Saadabi & Zaid, 2011) results that reported that the extracts of *moringaoleifera* have an impeding effect on pathogenic bacteria like *Pseudomonas aeruginosain* and *Escherichia coli* (Saadabi & Zaid, 2011). The result of this study concludes that ethanol extracts of *moringaoleifera* showed a maximum zone of inhibition (17 mm) against *Pseudomo-*

nas aeruginosainas in (Table 2). This conclusion also describes the study by (Al-Bakri & Afifi, 2007) who mentioned moringa leaf extract constraining the growth of *E. coli*, *Klebsiella pneumoniae*, and *P.aeruginosa* (Al-Bakri & Afifi, 2007). Numerous investigations have shown that *M. oleifera* leaves have antibacterial properties. As an illustration, a study on plant extracts prepared in different solvents found the ether extract of leaves of *M. oleifera* was the most active ingredient against the ambient and clinical isolates of *Proteus mirabilis*, a well-known cause of urinary tract infections (Arun & Rao., 2001). Several studies on the antifungal activity of *M. oleifera* leaves against *Trichophytonrubrum*, *T. mentagrophytes*, *Epidermophytonfloccosum*, and *Microsporum* documented that the crude extracts as well as essential oils from *M. oleifera* leaves reveal antifungal activity (Abalaka et al., 2012; Chuang et al., 2007). (Patel et al., 2014) study showed *M. oleifera* leaf extracts in ethanolic and aqueous forms were effective against the yeast *Saccharomyces cerevisiae* and the fungus *Candida tropicalis*, but not against *C. albicans*. Little is known about the antibacterial activity of *M. oleifera* roots. Nevertheless, a few investigations have revealed this plant's roots to have anti-microbial properties (Patel et al., 2014). Additionally, in vitro tests on several *M. oleifera* root bark extracts against *S. aureus*, *E. coli*, *Salmonella gallinarum*, *P. aeruginosa*, and others showed that ethyl acetate and acetone extracts have the highest activity in comparison to other solvents (Raj et al., 2011). Similar to this, only a small amount of research—a few early reports—has been done on the antibacterial properties of *M. oleifera*'s stem bark. Studies demonstrate the existence of active organic extracts with variable degrees of activity in *M. oleifera* root extract's antibacterial efficacy against several human diseases (Chhetri et al., 2008).

CONCLUSION

The current study showed that *moringa oleifera* leaf extracts have an antibacterial activity that impedes bacterial growth. The results express that ethanol extract of *moringa oleifera* leaf is effective against bacterial strains.

The antibacterial effect may be due to bioactive constituents such as alkaloids, saponins, flavonoids, and tannins. Therefore, the study results emphasized the *moringa oleifera* leaf components and its therapeutic prospects as an antibacterial agent.

Duality of interest: In relation to this paper's publication, the authors state that they have no conflicts of interest.

Author contributions: Practical experimentation was conducted with Safa E. Rahuma assistance. Munira M. Ashrif contributed in writing, reviewing, and debating the paper.

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The Conduct of Statistical Models when Parameters Are Perturbed From Their True Values

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Abstract

This paper aims to investigate the so-called non-linear properties of the skeleton of a non-linear autoregressive process, i.e., if $X_t - f(X_{t-1}) = \varepsilon_t$. Setting the variance of $\varepsilon_t = 0$, the skeleton of the process is obtained. Having fitted a self-exciting threshold autoregressive (SETAR) model to data and obtained a 95% confidence interval for parameters, we study the behaviour of non-linear properties, e.g., a limit cycle, amplitude dependency frequency, etc. We mainly consider a limit cycle for values of parameters at various locations within the confidence interval, or we may just slightly perturb model parameters from their true values.

Keywords: SETAR models, A limit point, A limit cycle, Simulation.

INTRODUCTION

A Self-Exciting Threshold Autoregressive (SETAR) Model: Tong (1983) proposed a self-exciting threshold autoregressive (SETAR) Model in his study of river flow data, which takes the form

$$X_t = \begin{cases} b^{(1)}X_{t-1} + \varepsilon_t^{(1)} & \text{if } X_{t-d} \leq r \\ b^{(2)}X_{t-1} + \varepsilon_t^{(2)} & \text{if } X_{t-d} > r \end{cases} \quad (1)$$

where $\varepsilon_t^{(1)}, \varepsilon_t^{(2)}$ are each a strict white-noise process, $b^{(1)}, b^{(2)}$ are constants, and d the delay parameters, respectively. The multiple threshold model takes the formula

$$X_t = b^{(j)}X_{t-1} + \varepsilon_t^{(j)} \text{ if } X_{t-d} \in R^{(j)}; j = 1, 2, \dots, l$$

Where $R^{(1)}, R^{(2)}, \dots, R^{(l)}$ are given subset of the real line R , which define a partition of R into disjoint intervals $(-\infty, r_0], [r_0, r_1], \dots, [r_{l-1}, \infty)$, with $R^{(1)}$ denoting the interval $(-\infty, r_0]$ and $R^{(l)}$ denoting the interval $[r_{l-1}, \infty)$ (Priestley, 1988).

Jones and Cox (1978) discussed the general first order non-linear model



$$X_t - f(X_{t-1}) = \varepsilon_t \quad (2)$$

where $f(\cdot)$ is some general non-linear function, and ε_t is a sequence of independent variables. Model (1) can be used as a piecewise linear approximation to Model (2).

Similarly, a SETAR model of order $k > 1$ is given by

$$X_t = b_0^{(j)} + \sum_{i=1}^k b_i^{(j)} X_{t-i} + \varepsilon_t^{(j)} \text{ if } \underline{X}_{t-1} \in R^{(j)}; \quad j = 1, 2, \dots, l \quad (3)$$

Where $R^{(j)}$ is a given region of k -dimensional Euclidean space $R^{(k)}$, and $\underline{X}_{t-1} = (X_{t-1}, X_{t-2}, \dots, X_{t-k})^T$ is the state vector at time $t - 1$. Model (3) can be regarded as a piecewise linear approximation to the general k^{th} order non-linear AR model

$$\underline{X}_{t-1} - f(\underline{X}_{t-1}) = \varepsilon_t \quad (4)$$

A Limit Cycle: According to Tong (1983), a limit cycle in discrete time can be defined as follows: Given a non-linear difference equation $X_t - f(X_{t-1}) = 0$, here $X_t = (X_{t-1}, X_{t-2}, \dots, X_{t-p})$ is the state vector at time t , and f is a vector valued function, let $f^{(j)}$ denote the j^{th} iterate of f . Any vector of dimension p , which satisfies $f^{(jm)}(X) \rightarrow V$ as $j \rightarrow \infty$, is said to be a stable periodic point with a period m , with respect to domain $D \in R^p$. In this case $V_1, f^{(1)}(V_1), \dots, f^{(p-1)}(V_1)$, are all distinct stable limit points (Priestley, 1988).

The stable limit cycle is nothing but a set of vectors $(V_1, V_2, \dots, V_{p-1})$. A limit cycle does depend only on the parameter of the system and the initial conditions of the system. A limit cycle is said to be stable if it does not change with changing the initial conditions of the system. A stable limit cycle is the only one that can be observed in practice being one of the models of behaviour to which the system, then, it is said to be robust. A limit cycle with an infinite period is known as chaos, which is very dependent on the initial values of the system. SETAR models can give rise to a limit cycle behaviour where the white-noise is suppressed, or equivalently, when it has zero variance (Tong, 1990).

MATERIALS AND METHODS

A Simulation Study: The aim of this study is to see whether, if we slightly change the parameters of a model that is known to have a limit cycle of a specific period, over their 95% bootstrap confidence intervals, the model would still have a limit cycle with a reasonable period, or would a period vary considerably as parameter values wander over their bootstrap confidence intervals. We consider simulation on two well-known models due to Tong and Lim (1980), which are known to have stable limit cycles each of period 9. The two models are

$$X_t = \begin{cases} 0.62 + 1.25X_{t-1} - 0.43X_{t-2} + \varepsilon_t^{(1)} & \text{if } X_{t-2} \leq 3.25 \\ 2.25 + 1.52X_{t-1} - 1.24X_{t-2} + \varepsilon_t^{(2)} & \text{if } X_{t-2} > 3.25 \end{cases} \quad (5)$$

$$X_t = \begin{cases} 0.546 + 1.032X_{t-1} - 0.173X_{t-2} + 0.171X_{t-3} - 0.431X_{t-4} \\ + 0.332X_{t-5} - 0.284X_{t-6} + 0.210X_{t-7} + \varepsilon_t^{(1)} & \text{if } X_{t-2} \leq 3.16 \\ 2.632 + 1.492X_{t-1} - 1.32X_{t-2} + \varepsilon_t^{(2)} & \text{if } X_{t-2} > 3.16 \end{cases} \quad (6)$$

Our simulation consists of the following steps:

Step1. The bootstrap confidence interval of each parameter is constructed by using 50 replications, except for the delay parameter, where instead of constructing a bootstrap confidence interval, we allow the delay parameter to take the values 1, 2, 3, 4, and 5.

Step2. Starting from the lower limit of the bootstrap confidence interval of each parameter, and increasing by values, we simulate 1000 observations from each one of the skeletons of Models 5 and 6. The last 1000 observations are tested for a limit cycle with a possible maximum period of up to 500.

Step3. The experiment is terminated when the new perturbed value of each parameter reaches roughly the upper limit of its bootstrap confidence interval.

Step4. The above steps were repeated for each parameter in the skeleton of Models 5 and 6.

We could, if we wished, instead of constructing the bootstrap confidence interval of each parameter in Step 1, just perturb the model parameters from their true value; therefore, Step 1 is not an essential step.

It should be mentioned that, in this study, we do not investigate each limit cycle in detail (i.e., how many sub-limit cycles it has or whether it is stable or not). We mainly investigate the existence of a limit cycle and its period. In cases where a no-limit cycle of a period less than or equal to 500 exists, we assume either it has a period greater than 500, or it is a chaos.

RESULTS

The value of each parameter, as it wanders over roughly its 95% bootstrap confidence interval, and the period of the corresponding limit cycle (if any) are given in Tables 1 to 7. Cases, where no limit cycle of a period less than, or equal to, 500 exists are denoted by *.

When the same limit cycle occurs in a sub-interval rather than at a single point within the bootstrap confidence interval of each parameter, the lower and upper limits of the sub-interval are given in each table. A single point is given as a sub-interval with equal upper and lower limits. Due to the

similarity in the results for Models (5-6) and the lack of space, we give here only the results for Model 5. The other results can be obtained from the authors.

Table: (1). The limit cycles occurred due to small changes in the constant-term in the first region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
0.474		0.584	1
0.585		0.585	12
0.586		0.588	11
0.589		0.592	10
0.593		0.600	9
0.601		0.610	8
0.611		0.638	9
0.639		0.739	8

Table: (2). The limit cycles occurred due to small changes in the first-coefficient in the first region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
1.202		1.238	1
1.239		1.239	13
1.240		1.241	10
1.242		1.243	9
1.244		1.247	8
1.248		1.257	9
1.258		1.310	8
1.311		1.363	9

Table: (3). The limit cycles occurred due to small changes in the second-coefficient in the first region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
-0.597		-0.464	1
-0.463		-0.463	25
-0.462		-0.462	12
-0.461		-0.461	77
-0.460		-0.450	*
-0.449		-0.417	9

Table:(4). The limit cycles occurred due to small changes in the constant-term in the second region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		UpperLimit	
2.134		2.214	8
2.215		2.274	9
2.275		2.364	8
2.365		2.374	51
2.375		2.474	*
2.475		2.484	98
2.485		2.494	144
2.495		2.504	169
2.505		2.514	103
2.515		2.524	81
2.525		2.534	47
2.535		2.574	12

Table:(5). The limit cycles occurred due to small changes in the first-coefficient in the second region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
1.340		1.410	10
1.411		1.484	9
1.485		1.510	8
1.511		1.530	9
1.531		1.553	8
1.554		1.554	34
1.555		1.555	51
1.556		1.556	17
1.557		1.557	70
1.558		1.566	*

Table: (6). The limit cycles occurred due to small changes in the second-coefficient in the second region for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
-1.367		-1.343	10
-1.342		-1.275	9
-1.274		-1.250	8
-1.249		-1.231	9
-1.230		-1.205	8
-1.204		-1.204	25
-1.203		-1.203	442
-1.202		-1.193	*

Table: (7). The limit cycles occurred due to small changes in the threshold value in for the skeleton of Model 5.

Bootstrap	Confidence	Interval	Period
Lower Limit		Upper Limit	
3.184		3.218	8
3.219		3.273	9
3.274		3.312	8
3.313		3.363	9
3.364		3.405	10
3.406		3.431	11
3.432		3.445	12
3.446		3.451	13
3.452		3.452	14
3.453		3.461	1

DISCUSSION

Examination of Tables 1–7 drew the following conclusion:

- 1). The most frequent limit cycles that occur are the original limit cycle of the models that has a period of 9 and limit cycles with periods of a multiple of 9 or with periods close to 9.
- 2). The two models appear to retain the original limit cycle of period 9 in the neighbourhood of each true parameter value, which suggests that the original limit cycle of each one of the two models is robust.
- 3). Model 5 appears to be more sensitive to minor changes in some parameters than others.
- 4). Where the same limit cycle is exhibited among the sub-intervals within the bootstrap confidence interval of each parameter, the ones where the original limit cycle occurred are the largest.

CONCLUSION

It should be noted that these results are specific to Model 5. Moreover, we have used only one initial value in simulated data from the skeletons of Model 5, which does not guarantee the stability of the limit cycles found during the experiment.

For future work, we suggest using more models with different initial values before these results can be generalized. In addition, it would be interesting to repeat this study using skeletons of bootstrap models rather than skeletons of initial models like the ones adopted in our experiment. In other words, it would be attractive to see if fitted, a SETAR model gave rise to a limit cycle behaviour of a specific period, whether the corresponding bootstrap model would give rise to the same limit cycle, and how sensitive it is to small changes in the bootstrap model parameters.

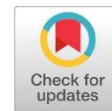
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On β -Generalized Open and Closed Sets in Neutrosophic Topological Spaces

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Abstract

This article demonstrates a class of neutrosophic closed sets named neutrosophic generalized βg -closed sets, discusses their essential characteristics in neutrosophic topological spaces, and analyses some new interesting theorems based on the newly introduced set. It also discusses its relationship between basic open and closed sets in neutrosophic topological spaces.

Keywords: Neutrosophic sets, neutrosophic topology, neutrosophic generalized βg -closed sets, and neutrosophic generalized βg -open sets.

INTRODUCTION

The concept of neutrosophic sets was first introduced by Floretin Smarandache (Floretin S.2010) in 1999, which is a generalization of intuitionistic fuzzy sets by Atanassov (Atanassov K. 1986). In (Dhavaseelan R. & Jafari S.2017), a generalized neutrosophic closed set (in short, N_gCS) is defined, and using this generalized neutrosophic continuous, generalized neutrosophic irresolute functions are defined.

Recently in (Dhavaseelan R., Jafari S. & Hani Md. 2018, Dhavaseelan R. & Hani Md. 2019), the perception of generalized α -contra continuous and neutrosophic almost α -contra-continuous functions are introduced.

In 1999, the neutrosophic sets and neutrosophic topological spaces by Salama A. A. and Alblowi S. A. were extended (Rena T. & Anila S.2018). Furthermore, the basic sets like neutrosophic open sets (NOS), neutrosophic semiopen sets (NSOS) neutrosophic pre-open sets (NPOS), neutrosophic α open sets ($N_\alpha OS$), neutrosophic regular open sets (N-ROS), neutrosophic β open sets ($N_\beta OS$), and neutrosophic b open sets (N-bOS) are introduced in neutrosophic topological spaces and their properties are studied by various authors (Pushpaiatha A.& Nandhini T.2019). This paper introduces the new concept of neutrosophic closed sets called generalized neutrosophic β closed and open sets and some of their basic properties with examples.

1- PRELIMINARIES:

In the following section, we assume that (X, τ) is the neutrosophic topological space, let A be a neutrosophic set in X and it is an open set. Then we symbolize it by $NSO(A)$, and the com-



plement of A is termed a neutrosophic closed set in X , also symbolized by $NSC(A)$. Also, the neutrosophic interior is denoted by $Nint(A)$, neutrosophic closure is denoted by $Ncl(A)$, and the empty band whole sets are denoted by 0 & 1 respectively.

Definition 1.1 (Abd El Monsef M.E. 1980)

A sub set A of topological space (X, τ) is called β – open (or semi pre open [6] if $A \subset cl(int(cl(A)))$.

Definition 1.2 (Levine N. 1970)

A sub set A of topological space (X, τ) is called a generalized closed set (g – closed for short) if $cl(A) \subseteq U$, whenever $A \subseteq U$ and U is an open set. The complement of g – closed set is called a g – open set.

Definition 1.3 (Dunham W. 1982)

If A is a subset of a space (X, τ) , then

- 1- The generalized closure of A is defined as the intersection of all g – closed sets in X containing A and is denoted by $gcl(A)$ where $gcl(A) = \bigcap \{F : F \text{ is } g\text{-closed} \& A \subseteq F\}$.
- 2- The generalized interior of A is defined as the union of all g – open sets in X contained in A and is denoted by $gint(A)$ where $gint(A) = \bigcup \{G : G \text{ is } g\text{-open} \& G \subseteq A\}$.

Definition 1.4 (Pushpaiatha A. & Nandhini T. 2019)

For subset A of topological space (X, τ) , then

- 1- The β – closure of A is the intersection of all β – closed set that contain A . They are denoted by $\beta cl(A)$.
- 2- The β – interior of A is the union of all β – open sets contained in A . They are denoted by $\beta int(A)$.

Definition 1.5 (Salama A.A. & Alblowi S.A. 2012)

Let X be a non-empty fixed set, A neutrosophic set $NS - (A)$ is an object having the form $A = \{\langle X, \mu_A(x), \delta_A(x), V_A(x) \rangle : x \in X\}$ where $\mu_A(x)$, $\delta_A(x)$ & $V_A(x)$ represent the degree of membership, degree of indeterminacy, and the degree of nonmembership respectively of each element $x \in X$ to the set A . A

neutrosophic set

$A = \{\langle X, \mu_A(x), \delta_A(x), V_A(x) \rangle : x \in X\}$ can be identified as an ordered triple $\langle \mu_A, \delta_A, V_A \rangle$ in $]0, 1[$ or X .

Definition 1.6 (Salama A.A. and Alblowi S.A. 2012)

Let $A = \langle \mu_A, \delta_A, V_A \rangle$ be a NS on X , then the complement $C(A)$ may be defined as

- 1- $C(A) = \{\langle x, 1 - \mu_A(x), 1 - \delta_A(x), 1 - V_A(x) \rangle : x \in X\}$.
- 2- $C(A) = \{\langle x, V_A(x), \delta_A(x), \mu_A(x) \rangle : x \in X\}$.
- 3- $C(A) = \{\langle x, V_A(x), 1 - \delta_A(x), \mu_A(x) \rangle : x \in X\}$.

Note that for any two neutrosophic sets A & B

$$4- C(A \cup B) = C(A) \cap C(B).$$

$$5- C(A \cap B) = C(A) \cup C(B).$$

Definition 1.7 (Salama A.A. & Alblowi S.A. 2012)

For any two neutrosophic sets

$$A = \{(x, \mu_A(x), \delta_A(x), V_A(x)) : x \in X\}, \text{ and}$$

$$B = \{(x, \mu_B(x), \delta_B(x), V_B(x)) : x \in X\} \text{ we may have}$$

$$1- A \subseteq B \Leftrightarrow \mu_A(x) \leq \mu_B(x),$$

$$\delta_A(x) \geq \delta_B(x), V_A(x) \geq V_B(x), \forall x \in X.$$

2-

$$A \cap B =$$

$$\langle x, \mu_A(x) \wedge \mu_B(x), \delta_A(x) \vee \delta_B(x), V_A(x) \vee V_B(x) \rangle$$

3-

$$A \cup B =$$

$$\langle x, \mu_A(x) \vee \mu_B(x), \delta_A(x) \wedge \delta_B(x), V_A(x) \wedge V_B(x) \rangle$$

Definition 1.8 (Salama A.A. and Alblowi S.A. 2012)

A neutrosophic topology (in short, NT) on

$X \neq \emptyset$ is a family τ of N -sets in X satisfying the laws given below

$$1- 0_N, 1_N \in \tau.$$

$$2- W_1 \cap W_2 \in \tau \text{ being } W_1, W_2 \in \tau.$$

$$3- \bigcup W_i \in \tau \text{ for the arbitrary family}$$

$$\{W_i : i \in A\} \subseteq \tau.$$

In this case the pair (X, τ) is a neutrosophic topological space (NTS) and any neutrosophic set in τ is known as a neutrosophic open set (NOS) in X . A neutrosophic set A is a neutrosophic closed set (NCS) if and only if its complement $C(A)$ is a neutrosophic open set in X .

Definition 1.9

A neutrosophic A in a neutrosophic topological space (X, τ) is said to be

$$1- \text{A neutrosophic } \beta\text{-open set } (N_\beta OS) \text{ if } A \subseteq Ncl(Nint(Ncl(A))).$$

$$2- \text{A neutrosophic } \beta\text{-closed set } (N_\beta CS) \text{ if } Nint(Ncl(Nint(A))) \subseteq A.$$

Remark 1.1

Note that $Ncl(C(A)) = C(Nint(A))$ &

$$Nint(C(A)) = C(Ncl(A)).$$

Proposition 1.1 (Salama A.A. and Alblowi S.A. 2012)

Let (X, τ) be NTS and A, B be two neutrosophic sets in X , then the following properties hold:

$$(a) Nint(A) \subseteq A, \quad (b) A \subseteq Ncl(A),$$

$$(c) A \subseteq B \Rightarrow Nint(A) \subseteq Nint(B),$$

$$(d) A \subseteq B \Rightarrow Ncl(A) \subseteq Ncl(B),$$

$$(e) Nint(Nint(A)) = Nint(A) \wedge Nint(B), \quad (f) Ncl(A \cup B) = Ncl(A) \vee Ncl(B),$$

$$(g) Nint(1_N) = 1_N, \quad (h) Ncl(0_N) = 0_N.$$

Proposition 1.2 (Salama A.A. & Alblowi S.A. 2012)

For any neutrosophic set A in (X, τ) we have

- (a) $Ncl(C(A)) = C(Nint(A))$,
- (b) $Nint(C(A)) = C(Ncl(A))$.

Proposition 1.3 (Salama A.A. & Alblowi S.A. 2012),

For all, A, B two neutrosophic sets then the following are true

- (a) $C(A \cap B) = C(A) \cup C(B)$,
- (b) $C(A \cup B) = C(A) \cap C(B)$.

Definition 1.10 (Salama A.A. & Alblowi S.A. 2012)

Let A be an NS in an $NTS (X, \tau)$, there for

1-

$$Nint(A) = \bigcup \{G : G \text{ is a NOS in } X \text{ and } G \subseteq A\}$$

is termed as neutrosophic interior ($Nint$ for short) of A .

2-

$$Ncl(A) = \bigcap \{G : G \text{ is an NCS in } X \text{ and } G \supseteq A\}$$

is termed as neutrosophic closure (Ncl for short) of A .

Definition 1.11 (Pushpaiatha A. & Nandhini T. 2019)

A NS A in $NTS X$ is so called a neutrosophic generalized closed set denoted by

N_gCS if for any NOS U in X such that

$A \subseteq U$, then $Ncl(A) \subseteq U$. Moreover, its complement is named a neutrosophic generalized open set and referred to N_gOS .

Definition 1.12 (Dhavaseelan R. & Jafari S. 2017)

Let (X, τ) be NTS and B be a NS in X , then neutrosophic generalized closure is defined as

$$N_gcl(B) = \bigcap \{G : G \text{ is a GNCS in } X \text{ and } B \subseteq G\}$$

$$N_gint(B) =$$

$$\bigcup \{U : U \text{ is a GNOS in } X \text{ and } U \subseteq B\}$$

Proposition 1.4 (Salama A.A. & Alblowi S.A. 2012),

For any generalized neutrosophic set A

the following are holds:

$$0_N \subseteq A, \quad 0_N \subseteq 0_N, \quad A \subseteq 1_N, \quad 1_N \subseteq 1_N$$

Proposition 1.5 (Salama A.A. & Alblowi S.A. 2012)

Let (X, τ) be a $GNTS$ and A, B be two neutrosophic sets in X . Then the following properties hold:

- (a) $Gint(A) \subseteq A$, (b) $A \subseteq GNcl(A)$, (c) $A \subseteq B \Rightarrow GNint(A) \subseteq GNint(B)$,
- (d) $A \subseteq B \Rightarrow GNcl(A) \subseteq GNcl(B)$,
- (e) $GNint((A \cap B)) = GNint(A) \wedge GNint(B)$,

- (f) $GNcl((A \cup B)) = GNcl(A) \vee GNcl(B)$,
 (g) $GNint(1_N) = 1_N$, $GNcl(0_N) = 0_N$.

Proposition 1.6 (Salama A.A.& Alblowi S.A. 2012)

For any generalized neutrosophic set A in (X, τ) we have

- (a) $GNcl(C(A)) = C(GNint(A))$,
 (b) $GNint(C(A)) = C(GNcl(A))$.

Definition 1.13

Let A be a neutrosophic set of a neutrosophic topological space (X, τ) , then the neutrosophic β -interior and the neutrosophic β -closure are defined as

$$N_{\beta}int(A) = \cup \{U : U \text{ is } N\beta OS \text{ in } X \text{ \& } U \subseteq A \},$$

$$N_{\beta}cl(A) = \cap \{F : F \text{ is } N\beta CS \text{ in } X \text{ \& } A \subseteq F\}.$$

Proposition 1.7

Let A be an a neutrosophic set in X , then

- 1- $N_{\beta}cl(A) = A \cup Nint(Ncl(Nint(A)))$.
 2- $N_{\beta}int(A) = A \cap Ncl(Nint(Ncl(A)))$.

Proof:

- 1- We need to prove that $N_{\beta}cl(A) \subseteq A \cup Nint(Ncl(Nint(A)))$ &

$$A \cup Nint(Ncl(Nint(A))) \subseteq N_{\beta}cl(A)$$

$$\text{Since } N_{\beta}cl(A) \subseteq N_{\beta}CS(A) \Rightarrow$$

$$Nint(Ncl(Nint(N_{\beta}cl(A)))) \subseteq N_{\beta}cl(A)$$

$$\Rightarrow A \cup Nint(Ncl(Nint(A)))$$

$$\subseteq A \cup Nint(Ncl(Nint(N_{\beta}cl(A))))$$

$$\subseteq A \cup N_{\beta}cl(A) = N_{\beta}cl(A). \quad \rightarrow (1)$$

On the other hand, since we have

$$Nint(Ncl(Nint((A)))) \cup$$

$$Nint(Ncl(Nint((A))))$$

$$\subseteq Nint(Ncl(Nint((A \cup Ncl(A))))$$

$$= Nint(Ncl(Nint(Ncl(A))))$$

$$= Nint(Ncl(Nint((A))))$$

$$\subseteq A \cup Nint(Ncl(Nint((A)))) \rightarrow (2)$$

From (1) & (1) we get

$$N_{\beta}cl(A) = A \cup Nint(Ncl(Nint(A))).$$

2- The proof of this case similar to paragraph 1.

2- β - Generalized Closed and Open Sets in Neutrosophic Topological Spaces:

In this section we introduce concepts of the neutrosophic closure, neutrosophic- β interior and β -generalized closed and open sets and its respective open set in neutrosophic topological spaces and discuss some of their properties.

Definition 2.1 (Rukaia M. Rashed 2020)

A sub set A of a topological space (X, τ) is called a β -generalized closed set ($g\beta$ -closed) if $\beta cl(A) \subseteq U$ whenever $A \subseteq U$ and $U \in \beta O(X)$.

Definition 2.2 (Rukaia M. Rashed 2020)

A subset A of a topological space (X, τ) is said to be a generalized β -open ($g\beta$ -open for short) set if $U \subseteq \beta int(A)$ where ever $U \subseteq A$ and U is closed. The complement of generalized β -open set is said to be generalized β -closed. The family of all $g\beta$ -open (resp. $g\beta$ -closed) sets of X is denoted by $G\beta O(X)$ (resp. $PG\beta C(X)$).

Proposition 2.1

Let (X, τ) be a neutrosophic topological space, then the union of any two $N_{\beta}OS$ in a $NTSX$ is a $N_{\beta}OS$.

Proof:

Let A & B be two $N_{\beta}OS$, therefore

$$A \subseteq Ncl(Nint(Ncl(A))) \text{ \& }$$

$$B \subseteq Ncl(Nint(Ncl(B))) \Rightarrow$$

$$A \cup B \subseteq$$

$$Ncl(Nint(Ncl(A))) \cup Ncl(Nint(Ncl(B)))$$

$$= Ncl(Nint(Ncl(A) \cup Ncl(B)))$$

$$\subseteq Ncl(Nint(Ncl(A) \cup Ncl(B)))$$

$$= Ncl(Nint(Ncl(A \cup B))), \text{ then}$$

$$A \cup B \subseteq Ncl(Nint(Ncl(A \cup B))),$$

so that $A \cup B$ is a $N_{\beta}OS$ in X .

Remark 2.1

The intersection of any two $N_{\beta}OS$ of an NTS does not have to be a $N_{\beta}OS$ as in this example.

Example 2.1

Let $X = \{a, b\}$ & $\tau = \{0_N, 1_N, A, B, M, N\}$ is a NTS on X where

$$A = \langle x, (.3, .4), (.2, .1), (.7, .5) \rangle,$$

$$B = \langle x, (.2, .5), (.3, .4), (.4, .5) \rangle,$$

$$M = \langle x, (.3, .5), (.3, .4), (.4, .5) \rangle,$$

$$N = \langle x, (.2, .4), (.2, .1), (.7, .5) \rangle, \text{ and let}$$

$K_1 = \langle x, (.8, .4), (.1, .2), (.5, .7) \rangle,$
 $K_2 = \langle x, (.5, .6), (.2, .5), (.3, .3) \rangle.$ Then $Ncl(Nint(Ncl(K_1))) = 1_N,$
 $Ncl(Nint(Ncl(K_2))) = 1_N,$ therefor
 K_1 & K_2 are $N_\beta OS$ in X . But
 $K_1 \cap K_2 = \langle x, (.5, .4), (.1, .2), (.5, .7) \rangle$ is
 not $N_\beta OS$ in X .

Proposition 2.2

Let A be any neutrosophic set in a neutrosophic topological space X , and let $A \subseteq B \subseteq Ncl(A)$, then B is a $N_\beta OS$ set in X .

Proof:

Since A is a $N_\beta OS$ set so that
 $A \subseteq Ncl(Nint(Ncl(A))) \Rightarrow$
 $Ncl(A) \subseteq Ncl(Ncl(Nint(Ncl(A))))$
 $= Ncl(Nint(Ncl(A))) \Rightarrow$
 $Ncl(A) \subseteq Ncl(Nint(Ncl(A))),$ since
 $A \subseteq B \subseteq Ncl(A)$, then
 $B \subseteq Ncl(Nint(Ncl(A))).$ Also $A \subseteq B \Rightarrow$
 $Ncl(Nint(Ncl(A))) \subseteq Ncl(Nint(Ncl(B))),$
 hence $B \subseteq Ncl(Nint(Ncl(B))),$ then B is a $N_\beta OS$ set in X .

Proposition 2.3

Let (X, τ) be a neutrosophic topological space, and A be a neutrosophic set of X . Then A is $N_\beta CS$ if and only if $C(A)$ is a $N_\beta OS$.

Proof:

Suppose that A is a $N_\beta CS$ in X . Then $Nint(Ncl(Nint(A))) \subseteq A$, taking the compliment of both sides, then we have

$C(A) \subseteq C(Nint(Ncl(Nint(A)))) =$
 $Ncl(Nint(Ncl(C(A)))) \Rightarrow$
 $C(A) \subseteq Ncl(Nint(Ncl(C(A))))$, therefore
 $C(A)$ is $N_\beta OS$ in X .

On the other hand, suppose that $C(A)$ is $N_\beta OS$ in X . So that

$C(A) \subseteq Ncl(Nint(Ncl(C(A))))$, taking the complement of both sides we have

$$C \left(Ncl \left(Nint \left(Ncl(C(A)) \right) \right) \right) \subseteq A \Rightarrow \\ Nint \left(Ncl(Nint(A)) \right) \subseteq A.$$

Then A is a
 $N_\beta CS$ in X .

Proposition 2.4

The intersection of any two $N_\beta CS$ of an NTS , is also $N_\beta CS$.

Proof

Suppose that A & B are two $N_\beta CS$ in X . So $Nint \left(Ncl(Nint(A)) \right) \subseteq A$ &
 $Nint \left(Ncl(Nint(B)) \right) \subseteq B$, then
 $Nint \left(Ncl(Nint(A)) \right) \cap$
 $Nint \left(Ncl(Nint(B)) \right) \subseteq A \cap B \Rightarrow$
 $Nint \left(Ncl(Nint(A \cap B)) \right) \subseteq A \cap B$. Then
 $A \cap B$ is a $N_\beta CS$.

Remark 2.2

Note that the union of any two $N_\beta CS$ in X is not a $N_\beta CS$ as in the following example:

Example 2.2

Let $X = \{a\}$ & $\tau = \{0_N, 1_N, A, B\}$ be a
 NTS on X where $A = \langle x, (.2), (.5), (.3) \rangle$,
 $B = \langle x, (.1), (.5), (.7) \rangle$, and let
 $K_1 = \langle x, (.0), (.5), (.8) \rangle$,
 $K_2 = \langle x, (.1), (.2), (.3) \rangle$. Then
 $Nint(K_1) = 0_N$ & $Nint(K_2) = 0_N$.
Therefore, K_1 ,
 K_2 are $N_\beta CS$, but $K_1 \cup K_2$ is not $N_\beta CS$.

Proposition 2.5

Every NCS in X is a $N_\beta CS$.

Remark 2.3

The converse of the above proposition is not true in the general, as in the following example:

Example 2.3

Let $X = \{a, b, c\}$ & $\tau = \{0_N, 1_N, A, B\}$ is a NTS on X where
 $A = \langle x, (.5, .1, .1), (.6, .7, .6), (.3, .9, .4) \rangle$,
 $B = \langle x, (.0, .1, .5), (.4, .6, .5), (.7, .9, .8) \rangle$,
and let

$$K = \langle x, (.2, 0, .3), (.4, .2, .2), (.9, .9, .1) \rangle.$$

Then K is a $N_\beta CS$ but not a NCS .

Proposition 2.6

Let A be a $N_\beta CS$, and $Nint(A) \subseteq B \subseteq A$, then B is a $N_\beta CS$.

Proof

Suppose that A is a $N_\beta CS$, so

$$Nint(Ncl(Nint(A))) \subseteq A, \text{ then we have}$$

so $Nint(Ncl(Nint(A))) \subseteq Nint(A)$, and we have $Nint(A) \subseteq B$. Then, it follows that

$$Nint(Ncl(Nint(A))) \subseteq B, \text{ and } B \subseteq A \Rightarrow$$

$$Nint(Ncl(Nint(B))) \subseteq$$

$$Nint(Ncl(Nint(A))),$$

so $Nint(Ncl(Nint(B))) \subseteq B$, then B is a $N_\beta CS$.

Proposition 2.7

For any $NS A$ in $TS \tau$, the subsequent features stand:

- 1- $N_{\beta g}int(\bar{A}) = N_{\beta g}int(A)$.
- 2- $N_{\beta g}cl(\bar{A}) = N_{\beta g}cl(A)$.

Proof

The proof will be evident by symbolic definition,

$$Neg\beta cl(A) = \cap \{F: A \subseteq F, F \text{ is a } Ne - g\beta CS\}$$

$$1- Ne - g\beta cl(A) = \cap \{\bar{F}: \bar{A} \subseteq \bar{F}, \bar{F} \text{ is a } Ne - g\beta C(S)\}$$

$$= \cup \{U: A \supseteq U, U \text{ is a } Ne - g\beta OS\}$$

$$= Ne - g\beta int(\bar{A}).$$

2- This feature has undeniable proof analogous to feature (1).

Proposition 2.8

For any $N_{\beta g}OS A$ in $TS \tau$, then this set is $N_\beta OS$ (corresponding $N_{\beta g}OS$).

Proof

Similar to the proof of the previous theorem.

Definition 2.3

A neutrosophic A in a neutrosophic topological space X is said to be a neutrosophic β -generalized closed set ($N_{\beta g}CS$) if $N_{\beta g}cl(A) \subseteq U$ whenever $A \subseteq U$ and U is a NOS in X . The complement $C(A)$ of a $N_{\beta g}CSA$ is a $N_{\beta g}OS$ in X .

Definition 2.4

A neutrosophic A in a neutrosophic topological space X is said to be a neutrosophic β -generalized open set ($N_{\beta g}OS$) if

$U \subseteq N_{\beta}int(A)$ whenever $U \subseteq A$ and U is a N -closed set.

Example 2.4

Let $X = \{a, b\}$ and $\tau = \{0_N, 1_N, A, B\}$

where $A = \langle x, (.5, .6), (.3, .2), (.4, .1) \rangle$ &

$B = \langle x, (.4, .4), (.4, .3), (.5, .4) \rangle$ then τ is a neutrosophic topology. Hence let

$M = \langle x, (.5, .4), (.4, .4), (.4, .5) \rangle$ be any NS

in X then $M \subseteq A$ where A is a NOS in X . Now $N_{\beta}cl(M) =$

$\cap \{F : F \text{ is } N_{\beta}CS \text{ in } X \text{ \& } M \subseteq F\} = C(B) \subseteq A$, or $N_{\beta}cl(M) = M \cup C(B) = C(B) \subseteq A$.

Therefore M is a $N_{\beta g}CS$ in X .

$C(A) = \langle x, (.4, .1), (.3, .2), (.5, .6) \rangle$,

$C(B) = \langle x, (.5, .4), (.4, .3), (.4, .4) \rangle$, so A is

$N_{\beta}CS$ if $Nint(Ncl(Nint(A))) \subseteq A$

$\Rightarrow Nint(Ncl(Nint(A))) = o_N \subseteq A$,

also $Nint(Ncl(Nint(B))) = B \subseteq B$

$\Rightarrow A$ & B are neutrosophic β -closed sets.

Now, $N_{\beta}cl(M) = A \not\subseteq U = C(B)$, so that M is not $N_{\beta g}CS$.

Example 2.5

Let $X = \{a, b\}$, $\tau = \{0_N, 1_N, A, B\}$ is an

NTS , $A = \langle x, (.5, .3), (.5, .7), (.5, .7) \rangle$ &

$B = \langle x, (.4, .3), (.6, .7), (.6, .7) \rangle$ are NS in X , if $M = \langle x, (.4, .6), (.4, .4), (.4, .4) \rangle$, then M is

$N_{\beta g}CS$ but does not $N_{\beta}CS$ in X , since

$Nint(Ncl(Nint(M))) = A \not\subseteq M$.

Proposition 2.9

Every NCS A is a $N_{\beta g}CS$ in X but not conversely in general.

Proof

Let $A \subseteq U$ where U is a NOS in X ,

Now $N_{\beta}cl(A) = (N_{\beta}O(A))^c =$

$(A \subseteq Ncl(Nint(Ncl(A))))^c =$

$(A \subseteq Ncl(A))^c = (A \cup Ncl(A))^c =$

$(A \cup A)^c = A^c \subseteq U^c \Rightarrow A \subseteq U$,

by hypothesis therefore A is $N_{\beta g} - CS$.

Proposition 2.10

Every $N_{\beta}CS$ A is a $N_{\beta g}CS$ in X but the converse is not true in general.

Proof:

Let $A \subseteq U$, where A is $N_{\beta}CS$, U is a $N_{\beta}OS$ in X , then $N_{\beta}C(A) = (N_{\beta}O(A))^c$
 $= (A \subseteq Ncl(Nint(Ncl(A))))^c$
 $= N_{\beta}C(A) = A \subseteq U$ (by previous Proposition). Then we have $N_{\beta}C(A) \subseteq U$, hence A is an $N_{\beta_g}CS$ in X .

Proposition 2.11

Every $NOS, N_{\beta}OS$ are $N_{\beta_g}OS$ but not conversely in general.

Proof:

Obvious.

Remarks 2.4

1- The union of any two $N_{\beta_g}CS$ in a $NTSX$ is not a $N_{\beta_g}CS$ in a general case.

2- The intersection of any two $N_{\beta_g}CS$ need not be a $N_{\beta_g}CS$ in a $NTS X$ in general.

Example 2.7

Let $X = \{a, b\}$, and $\tau = \{0_N, 1_N, A, B, M\}$ be a neutrosophic topological space on X where $A = \langle x, (.5, .6), (.5, .4), (.5, .4) \rangle$ and $B = \langle x, (.2, .3), (.8, .7), (.8, .7) \rangle$, $M = \langle x, (.6, .7), (.4, .3), (.4, .3) \rangle$. Let $L_1 = \langle x, (.1, .5), (.9, .5), (.9, .5) \rangle$, $L_2 = \langle x, (.5, .2), (.5, .8), (.5, .8) \rangle$, then L_1 & L_2 are $N_{\beta_g}CS$ in X but $L_1 \cup L_2$ is not an $N_{\beta_g}CS$ since $L_1 \cup L_2 = \langle x, (.5, .5), (.5, .5), (.5, .5) \rangle \subseteq A$ but $N_{\beta}cl(L_1 \cup L_2) = \langle x, (.6, .7), (.4, .3), (.4, .3) \rangle \not\subseteq A$. Then M & N are $N_{\beta_g}CS$ in X but $M \cup N \subseteq B$ and $N_{\beta}cl(M \cup N) = 1_N \not\subseteq A$.

Example 2.8

Let $X = \{a, b\}$, and $\tau = \{0_N, 1_N, A, B, M\}$ is a neutrosophic topological space on X where $A = \langle x, (.5, .6), (.5, .4), (.5, .4) \rangle$ and $B = \langle x, (.2, .3), (.8, .7), (.8, .7) \rangle$, $M = \langle x, (.6, .7), (.4, .3), (.4, .3) \rangle$. Let $L_1 = \langle x, (.5, .8), (.5, .2), (.5, .2) \rangle$, $L_2 = \langle x, (.8, .6), (.2, .4), (.2, .4) \rangle$, then L_1 & L_2 are $N_{\beta_g}CS$ in X but $L_1 \cap L_2$ is not an $N_{\beta_g}CS$ since $L_1 \cap L_2 = \langle x, (.5, .6), (.5, .4), (.5, .4) \rangle \subseteq A$. But $N_{\beta}cl(L_1 \cap L_2) = \langle x, (.6, .7), (.4, .3), (.4, .3) \rangle \not\subseteq A$. Then M & N are $N_{\beta_g}CS$ in X but

$$M \cap N \subseteq B \text{ and } N_{\beta}cl(M \cap N) = 1_N \notin A.$$

Proposition 2.12

Let (X, τ) be a NTS . Then for every $A \in N_{\beta g}C(X)$ and for every $B \in NS(X)$, $A \subseteq B \subseteq N_{\beta}cl(A)$ implies that $B \in N_{\beta g}C(X)$.

Proof:

Let $B \subseteq U$ and U be a NOS in (X, τ) . Then, since $A \in N_{\beta g}C(X)$, $\Rightarrow N_{\beta}cl(A) \subseteq U$, $A \subseteq U$ then, since $B \subseteq N_{\beta}cl(A) \Rightarrow N_{\beta}cl(B) \subseteq N_{\beta}cl(N_{\beta}cl(A)) = N_{\beta}cl(A)$, so $N_{\beta}cl(B) \subseteq N_{\beta}cl(A) \subseteq U$, then $N_{\beta}cl(B) \subseteq U$, Hence $B \in N_{\beta g}C(X)$.

Example 2.9

Let $X = \{a, b\}$, $\tau = \{0_N, 1_N, A, B\}$, such that $A = \langle X, (.5, .5), (.5, .5), (.5, .5) \rangle$
 $B = \langle X, (.4, .3), (.6, .7), (.6, .7) \rangle$,
 $S = \langle X, (.3, .2), (.7, .8), (.7, .8) \rangle \Rightarrow S$ is $N_{\beta}CS$ in X , why? We have
 $C(A) = \langle X, (.5, .5), (.5, .5), (.5, .5) \rangle$,
 $C(B) = \langle X, (.6, .7), (.6, .7), (.4, .3) \rangle$,
 $C(S) = \langle X, (.7, .8), (.7, .8), (.3, .2) \rangle$ note that $C(S)S$ is not NCS , since $C(S) \notin \tau$.
 The $N_{\beta}OS$ are $A, B, C(A) \& C(B)$ since
 $A \subseteq Ncl(Nint(Ncl(A))) = C(A)$,
 $B \subseteq Ncl(Nint(Ncl(B))) = \langle X, (.5, .5), (.6, .7), (.5, .5) \rangle$,

$$C(A) \subseteq Ncl(Nint(Ncl(C(A)))) = C(A) \&$$

$$C(B) \subseteq Ncl(Nint(Ncl(C(B)))) = B.$$

The $N_{\beta}CS$ are $A, B, C(A) \& C(B)$, so that S is $N_{\beta g}CS$ if $N_{\beta}cl(S) \subseteq U$, U is $N_{\beta}OS$
 $N_{\beta}cl(S) = \cap \{K: K \text{ is a } N_{\beta}CS \text{ in } X \& S \subseteq K\} = A \cap B \cap C(A) \cap C(B) = B \Rightarrow S$
 is $N_{\beta g}CS$.

Proposition 2.13

If A is a NOS and a $N_{\beta g}CS$ in (X, τ) , then A is a $N_{\beta g}CS$ in (X, τ) .

Proof

Since $A \subseteq A$ and A is a NOS in (X, τ) , by hypothesis, $N_{\beta}cl(A) \subseteq A$. But $A \subseteq N_{\beta}cl(A)$. There $N_{\beta}cl(A) = A$. Hence A is a $N_{\beta}CS$ in (X, τ) .

Proposition 2.14

Every neutrosophic closed set in neutrosophic topological space (X, τ) is a neutrosophic generalized β -closed set.

Proof

Let A be a neutrosophic closed set in neutrosophic topological space X , let $A \subseteq U$ be a neutrosophic open set in X . Then by definition and previous proposition, we get $A = Ncl(A)$, $N_{\beta}cl(A) \subseteq Ncl(A)$, we get $N_{\beta}cl(A) \subseteq Ncl(A) = A \subseteq U$. Hence A is a neutrosophic generalized semi-closed set in X .

DISCUSSION

The results should be discussed in relation to any hypotheses advanced in the Introduction. Comment on results and indicate possible sources of error. Place the study in the context of other work reported in the literature. Only in exceptional cases should the "Results and Discussion" sections be combined. Refer to graphs, tables and figures by number (for example Figure 5 or Table 5. This helps tie the data into the text in a very effective manner.

CONCLUSION

This paper introduced and studied the notion of β -open and β -closed sets in a neutrosophic topology, and some characterizations of these notions are discussed. In future research, we will extend these neutrosophic topology concepts by neutrosophic generalized β -continuous and neutrosophic β -generalized continuous in neutrosophic topological spaces. Also, we extend this neutrosophic concept by nets, filters, and neutrosophic βg -compactnes.

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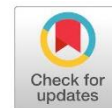
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Performance Evaluation of the Giga-bit 802.11ac Based WLANs

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Abstract

Wireless local area networks based on the legacy 802.11-1997 standard brought about a new era in wireless communications, enabling users to utilize the Internet anytime, anywhere. About two decades later, the IEEE 802.11ac amendment was released that broke the Gigabit-Ethernet barrier for wireless local area networks (WLANs). This amendment introduced improvements to the first and second layers (PHY and MAC) of the standard. The very high throughput was accomplished by improving the modulation mechanism, adding more spatial streams, utilizing broader channels, exploiting beam forming techniques, and allowing for better frame aggregation. In this article, a simulation evaluation is conducted to investigate the performance of the 802.11ac considering the enhancements introduced by this amendment. The main metric used in this study is the system throughput. In addition, the average delay metric is also considered for investigation. Different simulation scenarios are considered to examine the previously mentioned features and enhancements. Results showed that the system throughput of 802.11ac increases with larger channel sizes, improved modulation schemes, and more spatial streams. The frame aggregation has indicated to be an effective mechanism for alleviating unwanted overheads, which consequently increased the overall throughput.

Keywords: 802.11ac; modulation schemes; spatial streams; frame aggregation.

INTRODUCTION

Wireless communication technology offers the convenience of wireless communication services and enables individuals worldwide to stay mobile. Utilizing the IEEE 802.11 wireless standards, Wireless local area networks (WLANs) have undergone ongoing development year after year (Rochim *et al.*, 2020). WLANs are extensively utilized for various device types, with easy deployment options. Besides its usage in accessing the Internet, different applications use the WLANs, such as autonomous vehicles, surveillance, and audio/video delivery for real-time services. These applications involve users' mobility, which entails the probability of a high collision rate and potentially causing performance drops (Coronado *et al.*, 2023).

The data rates of the original 802.11 standard have been improved by the 802.11a/b/g amendments. The IEEE 802.11n standard was established in 2009, exploiting the MIMO technology that achieved higher throughput rounding to 0.6 Gbps. The IEEE 802.11ac (IEEE, 2013) amendment has succeeded in accomplishing a very high throughput (VHT), which exceeds the Giga-bit base-



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line. Accomplishing this VHT level was obtained according to several enhancements such as using more spatial streams, considering broader channels, increasing the modulation, and coding schemes, utilizing the new feature of multi-user MIMO, and frame aggregation techniques (IEEE, 2013).

Additionally, two essential frame aggregation methods are proposed by the amendment to be used by the MAC layer while transmitting data frames. These two methods are known as Aggregate MAC service data unit (A-MSDU) and Aggregate MAC protocol data unit (A-MPDU). The utilization of frame aggregation methods considerably decreases the overhead by allowing multiple frames to share the physical header and inter-frame spacing during channel access. Moreover, the frame size has increased, as stated by the amendment, to enable more data packets coming from upper layers to be aggregated. The frame aggregation mechanism, however, is set to be compulsory in 802.11ac, making the MAC layer transmits all its MPDUs as aggregate MPDUs (A-MPDUs) (Gast, 2013; IEEE, 2013).

Essentially, the 802.11ac builds upon the significant advancements made in 802.11n. Various techniques are employed in 802.11ac to increase data rates by utilizing MIMO technology. Instead of dealing with a single receiver, the 802.11ac proposed the MU-MIMO mechanism, which allows the access point to send to multiple users simultaneously. This is a groundbreaking feature that sets 802.11ac apart from its predecessors (Gast, 2013).

This paper aims to evaluate the new enhancements proposed by the 802.11ac and investigate their impact on the performance. Simulation methodology is utilized to conduct this study considering several scenarios which cover the features introduced in the 802.11ac. Broader channels, elevated modulation schemes, increased spatial streams, and frame aggregation are the enhancements investigated in this paper. Throughput and average delay are the metrics used in this study for performance evaluation. The evaluated performance indicated that the 802.11ac achieved better throughput when employing the new key features.

RELATED WORK

Extensive research has been proposed in the literature that investigated the operational effectiveness of the IEEE 802.11 wireless networks. Tuifaiga *et al.* presented a study that compares the performance of IEEE 802.11ac wireless LAN in Windows and Linux Ubuntu (Tuifaiga *et al.*, 2021). The study showed that IPv4 outperforms IPv6 in terms of several performance metrics. UDP has higher throughput than TCP, and Linux performs better than Windows. The theoretical limit of 1.3Gbps for 802.11ac was not reached with an 80 MHz channel size. Another study by (ElKassabi *et al.*, 2022) explored the practical deployment of WiFi standards in outdoor smart city environments. The study compared the 802.11ax, 802.11ac, and 802.11n in terms of performance. The results indicated that both IEEE 802.11ax and IEEE 802.11ac outperformed the performance of the IEEE 802.11n. Surprisingly, the distance between the transmitter and receiver was the criterion which made the 802.11ac perform better when a certain distance was exceeded. De Carvalho *et al.* evaluated the performance of wireless equipment in Wi-Fi (IEEE 802.11ac) using WPA2 PTP links (de Carvalho *et al.*, 2020). TCP and UDP performance metrics were measured. The 802.11ac outperformed 802.11n in terms of TCP throughput, jitter, and datagram loss. The results suggested further investigations across different standards, equipment, and environments. Alternatively, a Markovian model was presented to predict AP throughput based on network topology and demands (Stojanova *et al.*, 2021). Simulations showed a 10% mean error. The model is tailored for IEEE 802.11 standards with channel bonding, providing insights for channel assignment. Guidelines for static channel

bonding were derived considering node characteristics. The authors of (Natkaniec *et al.*, 2023) analyzed the coexistence of 802.11ax stations with other legacy stations. The study investigated the effect on system performance caused by the BSS coloring, A-MPDU, and A-MSDU aggregations. Simulation results showed that implementing BSS coloring increased throughput by up to 43%, but legacy devices disrupted its functioning. Fukuda *et al.* focused on IEEE 802.11ax and its impact on communication performance in dense campus wireless LANs (Fukuda *et al.*, 2022). They conducted experiments using multiple terminals to measure the throughput under various channel configurations and coexistence scenarios with other standards. Findings indicated that 40-MHz channel bonding improved throughput with a small number of terminals, whereas increasing the ratio of 802.11ax stations coexisting with 802.11ac stations enhanced the overall performance. The challenge of combining 802.11ad and 802.11ac interfaces in future WLAN devices was addressed by (Aggarwal *et al.*, 2022). The authors proposed MuSher, an agile MPTCP scheduler that improves throughput in WLAN/Internet settings and speeds up traffic recovery.

Similarly, Chen *et al.* focused on the challenges of rate adaptation (RA) in IEEE 802.11ac networks (Chen *et al.*, 2021). The authors identified limitations in current RA solutions, such as the lack of joint rate and bandwidth adaptation, scalability, and online learning capability. To overcome these limitations, they proposed an experience-driven rate adaptation (EDRA), which incorporates deep reinforcement learning. The evaluation results demonstrated that EDRA outperformed the default RAs by up to 821.4% (Intel) and 242.8% (Linux) in various scenarios. The research of (Khan *et al.*, 2017) discussed the high system throughput of IEEE 802.11ac networks in a MIMO channel. It considered key MAC and PHY layer features and identified trends and trade-offs. The work in (Muhammad *et al.*, 2021) presented a performance evaluation of 802.11ax (Wi-Fi 6). The research conducted empirical tests to investigate metrics such as throughput and jitter, and their relationship with parameters like payload length and environmental variables. The results showed that 802.11ax achieved higher throughput compared to its predecessor 802.11ac, and exhibited improved channel utilization due to its higher modulation and coding scheme. Confined to the 160-MHz channel, Kolahi *et al.* evaluated the performance of WLAN 802.11ac for IPv4, IPv6, UDP, and TCP protocols (Kolahi *et al.*, 2023). Results indicated that the client-server setup using UDP and IPv4 achieved the highest throughput at 1124 Mbps, surpassing the results for IPv6. However, the achieved throughput is lower than the theoretical maximum of 1700 Mbps. Another study (Gupta *et al.*, 2020) explored an integrated fiber-wireless network combining a 10-Gigabit passive optical network and IEEE 802.11ac WLAN. The focus was on enhancing network throughput and meeting quality of service requirements. The proposed approach incorporated a deficit dynamic bandwidth allocation algorithm at the optical line terminal to ensure improved QoS parameters. Simulation results demonstrated positive enhancements in all measured performance metrics. The authors of (Rochim *et al.*, 2020) compared the performance of the sixth-generation wireless protocol IEEE 802.11ax with the previous fifth-generation protocol IEEE 802.11ac, both operating at 5 GHz. Different modulation schemes and payload sizes, as well as the number of users, were considered for comparison. Results indicated that in the case of dense stations, 802.11ax performed better than 802.11ac. However, the 802.11ax experienced a slightly longer delay response time.

Buta *et al.* presented an implementation and evaluation of the sub-band MVDR algorithm for IEEE 802.11ac signals (Buta *et al.*, 2020). The algorithm demonstrated a good performance and effectively directed the array of antennas as required. Additionally, it improved data transmission quality, as indicated by lower bit error rates compared to non-beamforming scenarios under the same signal-to-noise ratio conditions. On the other hand, many studies focused on the impact of frame aggregation on network operation. Karmakar *et al.* conducted a survey examining the effect on application performance caused by the concepts of high throughput WLANs (Karmakar *et al.*, 2017). It covered

IEEE 802.11n and IEEE 802.11ac standards, highlighting features like frame aggregation, MIMO, and channel bonding. The survey emphasized the need for research on evaluating the performance of upper layers in HT-WLANs and developing efficient link adaptation mechanisms. The authors of (Suzuki *et al.*, 2021) proposed an optimization problem to maximize throughput in IEEE 802.11 networks using frame aggregation. They introduced a scheme that determined optimal subframe sets for both A-MPDU and A-MSDU, resulting in a significant improvement in throughput. Another work by (Yazid *et al.*, 2016) discussed the frame aggregation techniques and their effects on 802.11ac system performance. It also emphasized the importance of cross-layer communications between the PHY and MAC layers to optimize wireless bandwidth utilization. Simulation results demonstrated the benefits provided by the frame aggregation in improving network performance. Guo *et al.* focused on optimizing IEEE 802.11-based wireless networks, specifically for Linear Wireless Ad-hoc Networks (Guo *et al.*, 2022). The study identified the impact of the linear multi-hop characteristic on frame aggregation and the RTS/CTS handshake. Based on this analysis, a variable frame aggregation method and an adaptive RTS/CTS control algorithm were proposed to improve network performance in Linear-WANETs. Simulation results validated the effectiveness of the algorithm, demonstrating the significance of adjusting frame aggregation and RTS/CTS mechanisms to enhance overall system performance. Using simulations, the authors of (Khalil *et al.*, 2020) demonstrated that the 802.11ac standard could achieve throughputs of around 600 Mbit/s, approaching the data rates specified in the IEEE 802.11ac standard. The study presented the performance of hybrid frame aggregation, which achieved higher throughputs compared to A-MPDU or A-MSDU aggregations. Additionally, the study analyzed the most suitable modulation and coding schemes based on the distance between the station and the access point, finding that QPSK modulation performed better than 256-QAM for longer ranges.

MATERIALS AND METHODS

The Jemula 802.11ac simulator was used to assess the various aspects of 802.11ac (Jumela Team, 2016). It is an open-source Java library that serves as an event-driven stochastic simulation kernel for real-time systems. The simulator comprises three primary packages: kernel, statistics, and plot. Our simulation involved different channel configurations (20 MHz, 40 MHz, 80 MHz, and 160 MHz) and examined various modulation schemes, including QPSK, 16-QAM, 64-QAM, and 256-QAM. We also investigated the impact of varying the number of spatial streams (1, 2, 4, and 8). Table 1 summarizes the physical and MAC layer parameters (IEEE, 2013) as well as the frame aggregation parameters employed in the simulation. Multiple scenarios were created, with each scenario run for 20 seconds. The average values were obtained by executing every scenario for ten times to ensure the reliability and robustness of the obtained results.

Table:(1). Simulation Parameters.

Para.	Val.
Time of slot	9 μ s
CW _{min}	16
CW _{max}	1024
Prop Delay	1 μ s
TSIFS	16 μ s
TDIFS	34 μ s
MAC Header length	36 bits
Max MSDU length	2304 bytes
Max MPDU length	11454 bytes
BLK_ACK length	64 bytes
ACK length	14 bytes
Min P_HDR Time	40 μ s
Max P_HDR Time	68 μ s

RESULTS AND DISCUSSION

In this study, we intended to examine how various features implemented in 802.11ac impacted the overall throughput of the system. We assess the combined throughput of the network and evaluate the effects of these features utilizing different scenarios.

Scenario 1: Channel Bandwidth:

In order to investigate the impact of using broader channels, we vary the channel bandwidth, taking the values of 20, 40, 80, 160 MHz. The payload is also varied between 500 and 2000 octets. However, other parameters are fixed to focus only on the channel bandwidth effect. Modulation is fixed at 16-QAM, one spatial stream is used, and number of stations is set to 10. As shown in Figure 1, the system throughput increases by about 10 Mbps as the channel bandwidth is doubled. The increase in throughput can be interpreted easily when considering the formula of Shannon for channel capacity. That is when the bandwidth is widened, the channel can handle more data transfer, thus increasing the throughput. Nonetheless, another factor must be considered; the SNR, which plays a crucial role in the channel capacity formula.

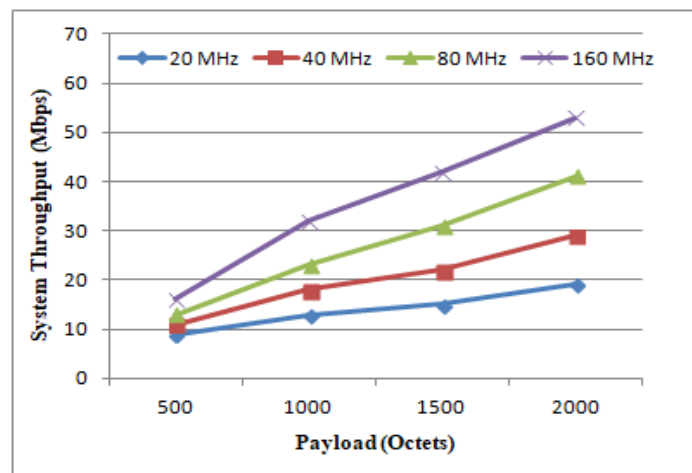


Figure: (1). Impact of channel bandwidth.

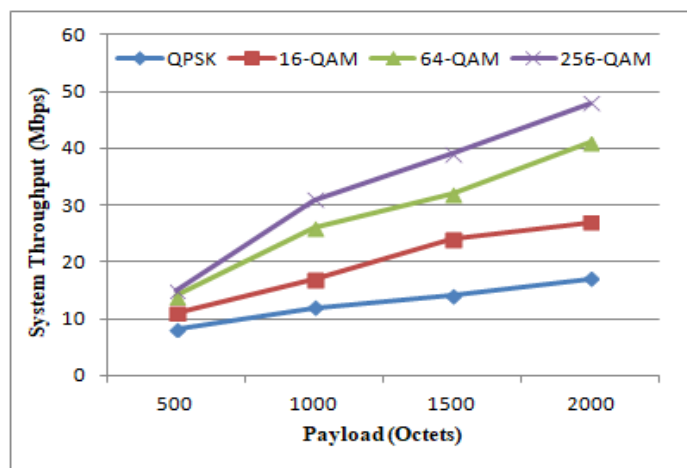


Figure: (2). Impact modulation schemes.

Scenario 2: Modulation Schemes

Modulation schemes are varied in this scenario (QPSK, 16-QAM, 64-QAM, and 256-QAM) to explore their influence on system throughput. For simplicity, we fix the spatial stream to one, the

number of stations is ten, and the channel bandwidth is 40 MHz. The system throughput increases with the increase of modulation and coding schemes, as illustrated in Figure 2. It is clearly understood and expected result because as the modulation scheme increases, the number of bits per symbol increases. This leads to conveying more data bits, which consequently increases the system throughput. It is worth to mention that the 256-QAM is newly proposed by the 802.11ac, which achieved about 10 Mbps higher than that of the 64-QAM.

Scenario 3: Spatial Streams

To evaluate the impact of spatial streams on system throughput, we varied the number of spatial streams with values 1, 2, 4, and 8 and plotted it against the payload size. We fixed the number of stations to 10, the modulation scheme is 16-QAM, and we used the 40 MHz channel. The system throughput is increased significantly with the increase of spatial streams, as depicted in Figure 3.

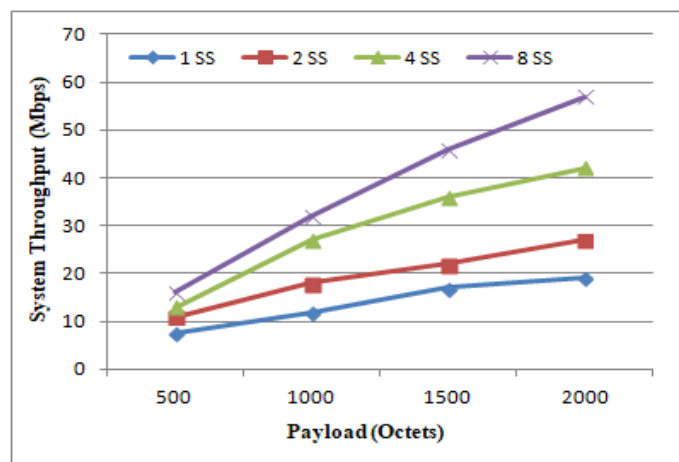


Figure: (3). Impact of spatial streams (SS).

It is clearly seen that the throughput is increased more than threefold when considering 8 spatial streams rather than 1 spatial stream. This is a great enhancement of the 802.11ac.

Scenario 4: MCS impact on average delay

Modulation and coding schemes are varied in this scenario to investigate the average delay in delivering data packets. Payload is fixed to 1500 octets, 20 MHz and 40 MHz channels are considered with spatial streams is set to 1. The average delay experienced by data transmission is decreased as the modulation and coding scheme increases, as shown in Figure 4. This decrement is observed in both channel bandwidths (20 and 40 MHz). However, the 40 MHz channel experiences a higher average delay than the 20 MHz channel. This can be attributed to the higher number of packets transmitted in case of using a wider channel.

Scenario 5: Impact of Frame Aggregation

The impact of employing the aggregate MPDUs is the aim of this scenario. We vary the number of the 2000 octets MPDUs that are aggregated into an A-MPDU. The 100 Mbps and 150 Mbps physical rates are used. The number of stations is fixed to 12 stations. The 40 MHz channel, along with 16-QAM is utilized. According to the results depicted in Figure 5, as the number of aggregated MPDUs increases, the throughput also increases. This can be taken as an evidence of the efficiency of frame aggregation mechanisms. This increase in throughput can be attributed to the reduction in the amount of overheads entailed by the MAC and PHY layers. However, after aggregating 64 or more MPDUs, the throughput reaches a plateau and no significant increase is observed. We argue

that when dealing with larger frames, higher physical rates are needed to accomplish better enhancements in system throughput.

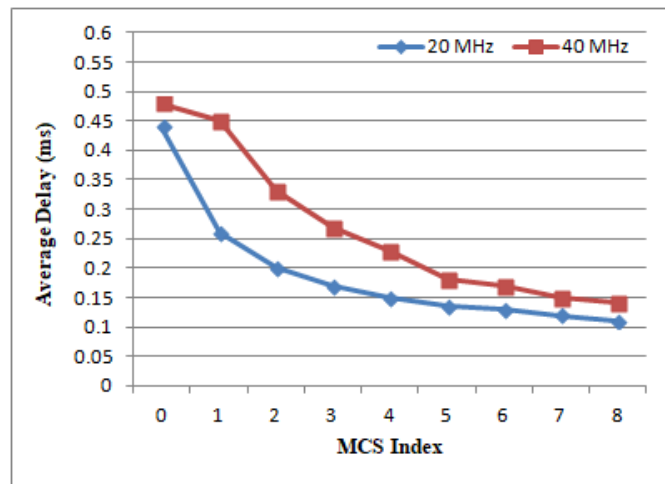


Figure: (4). Impact of MCS on average delay.

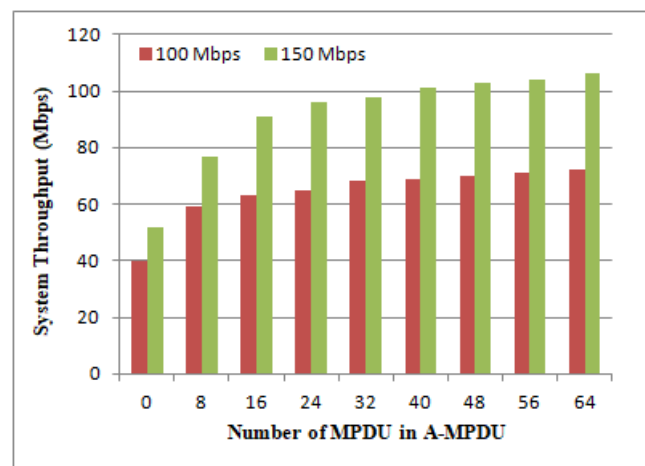


Figure: (5). Impact of Aggregate MPDU.

CONCLUSION

This study analyzed various aspects of the IEEE 802.11ac amendment. Our simulation scenarios focused on exploring wider channel bandwidths, modulation schemes, and multiple spatial streams, which are critical features of the amendment. The results demonstrated that these features significantly increase the system throughput, thereby improving overall performance. Additionally, we assessed the average delay as a metric to gain insights into the impact on data packet transmission. Based on simulation findings, it has been demonstrated that frame aggregation is a valuable approach for improving channel utilization. By reducing overhead, frame aggregation enhances the efficiency of the MAC protocol. However, it is essential to carefully consider the relationship between frame sizes and the physical data rate to ensure optimal performance.

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

Author contributions: Ashraf Bourawy brought up the research topic and conducted the simula-

tion scenarios. In addition, Abdalmonam contributed in setting up the simulation scenarios and parameters. Abdalmonam Abdalla surveyed the literature and wrote the introduction and related work. Ashraf Bourawy extracted the results and wrote the results and discussion part. Both authors contributed to the last version of the manuscript.

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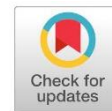
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Research Article

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A multi-step formable transform decomposition method for solving fractional order Riccati equation

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Abstract

A multi-step formable transform decomposition method (MFTDM) is suggested in this study to solve the nonlinear fractional-order Riccati problem. It is well understood that a corresponding numerical solution given by the FTDM is only valid for a short period. In the case of integer-order systems, however, the MFTDM solutions are more correct and reliable throughout time and are in very good agreement with the exact solutions. The fractional derivative is described in the Caputo sense. The method is tested on prominent examples, and the results show that it is accurate and efficient when compared to other numerical methods.

Keywords: Caputo derivative; Fractional order Riccati equation; Multi-step Formable transform decomposition Method.

INTRODUCTION

The formable transform decomposition method (FTDM) is a computational and analytical approach for solving fractional partial differential problems (Saadeh et al., 2023). The method provides the solution in terms of convergent series with easily computable components. In the past years, several academics have concentrated their efforts on the numerical solution of ordinary differential equations of fractional order and various numerical techniques, including the Fourier transform method (Kemle & Beyer, 1997), Homotopy perturbation method (Wang, 2007; Odibat & Momani, 2008; Mtawal & Alkaleeli, 2020), Homotopy analysis method (Canget al., 2009; Zurigat et al., 2010; Freihat, et al., 2014), Residual power series method (Ali et al., 2017), Alternative variational iteration method (Mtawalet al., 2020), Triple Shehu transform method (Alkaleeliet al., 2021; Kapooret al., 2022), the Laplace residual power series method (Burqan, et al., 2022). Recently, a formable transformation decomposition method (FTDM) was applied by (Al-ZouBi & Zurigat, 2014), it combines the formable integral transform (Saadeh, 2021) and the decomposition method (Momani & Al-Khaled, 2005; Shawagfeh, 2002; Khan et al., 2013; Mahdy et al., 2015). In the present study, we analyze the suitability and value of the MFTDM as a method to obtain the right approximation solutions to the fractional differential equation of the form using a series of intervals.

$$D_*^\beta y(t) = g(t) - L[y(t)] - N[y(t)], \quad (1)$$



with $t \geq 0$, $0 < \alpha \leq 1$, and subject to the initial condition.

$$y(0) = c. \quad (2)$$

Where $D_*^\beta y(t)$ is the fractional derivative of Caputo. This optimized approach is known as the multi-step formable transform decomposition method. The MFTDM was successfully shown to effectively, quickly, and accurately solve fractional differential equations. There is an enormous class of nonlinear fractional differential equations with approximations that rapidly converge to exact solutions. We provided two examples to show the effectiveness of our results.

PRELIMINARIES

This section describes the essential terminology and notations used in the fractional derivative field (Caputo, 1969; Miller & Roos, 1993; Beyer & Konuralp, 1995; Gorenflo & Mainardi, 1997; Podlubny, 1999). Also covered are the definition and characteristics of the formable integral transform (Kanwalet *al.*, 2018; Saadeh & Ghazal, 2021; Saadeh *et al.*, 2023).

Definition 2.1. The Riemann-Liouville fractional integral of order $\beta > 0$, of a function $f \in C_\rho$, $\rho \geq -1$ is defined as (Miller & Roos, 1993; Beyer & Konuralp, 1995; Gorenflo & Mainardi, 1997; Podlubny, 1999):

$$J^\beta f(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-\zeta)^{\beta-1} f(\zeta) d\zeta.$$

Definition 2.2. Let $f \in C_n^m$, $m \in \mathbb{N} \cup \{0\}$. The Caputo fractional derivative of f in the Caputo sense is defined as follows (Caputo, 1969):

$$D_t^\beta f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \int_0^t (t-\zeta)^{m-\beta-1} f^{(m)}(\zeta) d\zeta, & m-1 < \beta \leq m, \\ D_t^\beta f(t), & \beta = m. \end{cases}$$

Definition 2.3. (Saadeh & Ghazal, 2021; Saadeh *et al.*, 2023) A function $f : [0, \infty) \rightarrow \mathbb{R}$ is said to be of exponential order β ($\beta > 0$), if there $|f(t)| \leq M e^{\beta t}$, for all $t \geq t_0$.

Definition 2.4. The formable integral transform of a continuous function f on the interval $(0, \infty)$ is defined by (Saadeh & Ghazal, 2021; Saadeh *et al.*, 2023)

$$\begin{aligned} F[f(t)] &= \frac{s}{u} \int_0^\infty \exp\left(-\frac{st}{u}\right) f(t) dt \\ &= A(s, u). \end{aligned}$$

The formula for the inverse formable integral transform is

$$\begin{aligned} f(t) &= F^{-1}[A(s, u)] \\ &= \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{1}{s} \exp\left(\frac{st}{u}\right) A(s, u) ds. \end{aligned}$$

A constant's or polynomial's formable integral transform is given by:

$$F[a] = a.$$

$$F\left[t^m\right]=\left(\frac{u}{s}\right)^m m!, m \in N.$$

$$F\left[t^\beta\right]=\left(\frac{u}{s}\right)^\beta \Gamma(\beta+1), \beta>0.$$

Theorem 2.1. The Mittag-Leffler function's formable integral transform is provided by (Kanwalet al., 2018)

$$A(s, u) = \sum_{i=0}^{\infty} \lambda^i \left(\frac{u}{s}\right)^{\beta i + \alpha - 1}.$$

Theorem 2.2. Let f be a piecewise continuous function defined on $[0, \infty)$. Then, the formable integral transform of the Riemann-Liouville fractional integral of order $\beta > 0$ of the function f is given by (Saadeh & Ghazal, 2021; Saadehet al., 2023)

$$F\left[I_t^\beta f(t)\right] = \left(\frac{u}{s}\right)^\beta A(s, u).$$

Theorem 2.3. Let f be a piecewise continuous function defined on $[0, \infty)$. Then, the formable integral transform of the Caputo fractional derivative of the order β , $m-1 < \beta \leq m$, of the function f is given by (Saadeh & Ghazal, 2021; Saadehet al., 2023)

$$F\left[D_t^\beta f(t)\right] = \left(\frac{u}{s}\right)^\beta \left[A(s, u) - \sum_{i=0}^{m-1} \left(\frac{u}{s}\right)^i f^{(i)}(0)\right].$$

MATERIALS AND METHODS

Despite the fact that the FTDM (Saadeh, 2021) is used to approximate solutions to a wide range of nonlinear problems in terms of convergent series with readily calculated components, it has certain shortcomings: The series solution always converges rapidly in a small region and slowly in a bigger region. In this section, we present the core notions of the MFDTM that we built for numerically solving our problems (1) and (2). It is a simple tweak to regular FTDM that verifies the accuracy of the estimated solution for large time intervals. The solution is expanded over the interval $[0, t]$ by dividing it into i - subintervals $[t_{i-1}, t_i]$, $j = 1, 2, \dots, i$ of equal length Δt . If t^* is the initial value and $y_j(t)$ is an approximation in each subinterval $[t_{i-1}, t_i]$, $j = 1, 2, \dots, i$, the equations (1) and (2) can be transformed into the following system:

$$D_*^\beta y_j(t) = g(t) - L[y_j(t)] - N[y_j(t)], \quad (3)$$

with $t \geq 0$, $0 < \beta \leq 1$, $j = 1, 2, \dots, i$ and subject to the initial condition

$$y_j(t^*) = a, \quad y_j(t^*) = y_{j-1}(t_{j-1}) = c_j, \quad (4)$$

where $D_*^\beta y_j(t)$ is the Caputo fractional derivative, the source term is $g(t)$, L means the linear differential operator and N means the general nonlinear differential operator.

Using the formable integral (denoted by F in this study) on both sides of Equation (3), we obtain

$$F \left[D_*^\beta y_j(t) \right] = F \left[g(t) - L[y_j(t)] - N[y_j(t)] \right]. \quad (5)$$

Equation (5) can be read using Theorem 2.3 and the initial condition in equation (4) as

$$F[y_j(t)] = c_j + \left(\frac{u}{s}\right)^\beta F[g(t)] - L[y_j(t)] - N[y_j(t)]. \quad (6)$$

Using the formable inverse on both sides of Equation (6) yields

$$\begin{aligned} y_j(t) = & F^{-1}[c_j] \\ & + F^{-1} \left[\left(\frac{u}{s}\right)^\beta F[g(t)] - L[y_j(t)] \right] \\ & - F^{-1} \left[\left(\frac{u}{s}\right)^\beta F[N[y_j(t)]] \right]. \end{aligned} \quad (7)$$

Then,

$$y_j(t) = \sum_{i=0}^n y_{j,i}(t), \quad (8)$$

The nonlinear term in Equation (7) can be decomposed as follows:

$$N[y_{j,i}(t)] = \sum_{i=0}^{\infty} A_{j,i}(y_{j,0}, y_{j,1}, \dots, y_{j,i}), \quad (9)$$

for some Adomian's polynomials A_i that are given by (Ghorbani, 2009).

$$\begin{aligned} A_{j,i}(y_{j,0}, y_{j,1}, \dots, y_{j,i}) = \\ \frac{1}{i!} \left(\sum_{i=0}^n \frac{d^i}{d\lambda^i} N \left(\sum_{k=0}^{\infty} \lambda^k y_{j,k} \right) \right)_{\lambda=0}. \end{aligned} \quad (10)$$

Substituting Equations (8) and (9) into Equation (7) yields

$$\begin{aligned} \sum_{i=0}^n y_{j,i}(t) = & c_j + F^{-1} \left[\left(\frac{u}{s}\right)^\beta F[g(t)] \right] \\ & - F^{-1} \left[\left(\frac{u}{s}\right)^\beta F \left[\sum_{i=0}^{\infty} (L[y_{j,i-1}(t)]) \right] \right] \\ & - F^{-1} \left[\left(\frac{u}{s}\right)^\beta F \left[\sum_{i=0}^{\infty} (A_{j,i-1}) \right] \right]. \end{aligned} \quad (11)$$

After considering the comparison in Equation (11), we obtain

$$\begin{aligned}
y_{j,0}(t) &= c_j, \\
y_{j,1}(t) &= F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [g(t)] \right] \\
&\quad - F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [L[y_{j,0}(t)]] \right] \\
&\quad - F^{-1} \left[\left(\frac{u}{s} \right)^\beta f [A_{j,0}] \right], \\
y_{j,2}(t) &= -F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [L[y_{j,1}(t)]] \right] \\
&\quad - F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [A_{j,1}] \right], \\
&\vdots \\
y_{j,i}(t) &= -F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [L[y_{j,i-1}(t)]] \right] \\
&\quad - F^{-1} \left[\left(\frac{u}{s} \right)^\beta F [A_{j,i-1}] \right]. \quad (12)
\end{aligned}$$

In addition, a power series solution needs the form

$$y_j(t) = \sum_{i=0}^{\infty} y_{j,i}(t), \quad j = 1, 2, \dots, i. \quad (13)$$

Finally, the system (1) solutions have the form

$$y(t) = \begin{cases} y_1(t), & t \in [t_0, t_1], \\ y_2(t), & t \in [t_1, t_2], \\ \vdots & \\ y_i(t), & t \in [t_{i-1}, t_i]. \end{cases} \quad (14)$$

RESULTS

To show the applicability and effectiveness of our approach for solving nonlinear fractional Riccati equations, we explore the following examples: (Al-ZouBi&Zurigat, 2014; Zurigat et al., 2010; Canget al., 2009) :

Example 1. Consider the following nonlinear fractional Riccati equation

$$D_*^\beta y(t) = 1 - y^2(t), \quad t \geq 0, \quad 0 < \beta \leq 1, \quad (15)$$

with the initial condition

$$y(0) = 0. \quad (16)$$

The exact solutions of this equation when $\beta = 1$ is $y(t) = \frac{e^{2t} - 1}{e^{2t} + 1}$. If $y_j(t)$ is an approximation in each subinterval $[t_{i-1}, t_i]$, $j = 1, 2, \dots, i$, the equations (15) and (16) can be transformed into the following system:

$$D_*^\beta y_j(t) = 1 - y_j^2(t), \quad j = 1, 2, \dots, i. \quad (17) \quad y_j(t^*) = c_j, \quad (18)$$

With initial condition with $c_1 = 1$.

Using the formable integral (denoted by F in this study) on both sides of Equation (17), we obtain

$$F[D_*^\beta y_j(t)] = F[1 - y_j^2(t)], \quad (19)$$

Equation (19) can be read using Theorem 2.3 and the initial condition in equation (18) as

$$F[y_j(t)] = c_j + \left(\frac{u}{s}\right)^\beta F[1 - y_j^2(t)]. \quad (20)$$

Using the formable inverse on both sides of Equation (20) yields

$$y_j(t) = F^{-1}[c_j] + F^{-1}\left[\left(\frac{u}{s}\right)^\beta F[1 - y_j^2(t)]\right]. \quad (21)$$

Where $N[y_j(t)] = y_j^2(t)$ is a nonlinear operator, respectively. The nonlinear term of Eq.(21) can be decomposed as

$$N[y_j(t)] = y_j^2(t) = \sum_{i=0}^{\infty} A_{j,i}. \quad (22)$$

Adomian polynomials' first few components are provided by

$$\begin{aligned} A_{j,0} &= y_{j,0}^2, \\ A_{j,1} &= 2y_{j,0}y_{j,1}, \\ A_{j,2} &= 2y_{j,0}y_{j,2} + y_{j,1}^2, \\ &\vdots \end{aligned}$$

Assume that the solution of Equation (17) has the following series

$$y_j(t) = \sum_{i=0}^n y_{j,i}(t). \quad (23)$$

Substituting Equations (22) and (23) into Equation (21) yields

$$\sum_{i=0}^n y_{j,i}(t) = c_j + F^{-1}\left[\left(\frac{u}{s}\right)^\beta F\left[1 - \sum_{i=0}^{\infty} A_{j,i}\right]\right]. \quad (24)$$

After considering the comparison in Equation (24), we obtain

$$\begin{aligned} y_{j,0}(t) &= c_j, \\ y_{j,1}(t) &= F^{-1}\left[\left(\frac{u}{s}\right)^\beta F[1 - A_{j,0}]\right] \\ &= \frac{(1 - c_j^2)(t - t^*)^\beta}{\Gamma(\beta + 1)}, \\ y_{j,2}(t) &= -F^{-1}\left[\left(\frac{u}{s}\right)^\beta F[A_{j,1}]\right] \\ &= \frac{-2c_j(1 - c_j^2)(t - t^*)^{2\beta}}{\Gamma(2\beta + 1)}, \end{aligned}$$

$$\begin{aligned}
y_{j,3}(t) &= -F^{-1} \left[\left(\frac{u}{s} \right)^\beta F[A_{j,2}] \right] \\
&= \frac{4c_j^2 (1-c_j^2) (t-t^*)^{3\beta}}{\Gamma(3\beta+1)} \\
&\quad - \frac{(1-c_j^2)^2 \Gamma(2\alpha+1) (t-t^*)^{3\beta}}{\Gamma^2(\beta+1) \Gamma(3\beta+1)} \\
&\quad \vdots
\end{aligned} \tag{25}$$

The series solution to equation (17) is provided by

$$\begin{aligned}
y_j(t) &= c_j + \frac{(1-c_j^2) (t-t^*)^\beta}{\Gamma(\beta+1)} \\
&\quad - \frac{2c_j (1-c_j^2) (t-t^*)^{2\beta}}{\Gamma(2\beta+1)} + \frac{4c_j^2 (1-c_j^2) (t-t^*)^{3\beta}}{\Gamma(3\beta+1)} \\
&\quad - \frac{(1-c_j^2)^2 \Gamma(2\beta+1) (t-t^*)^{3\beta}}{\Gamma^2(\beta+1) \Gamma(3\beta+1)} + \dots
\end{aligned}$$

In this example, the suggested method is applied to the interval $[0, 10]$. We selected dividing the interval $[0, 10]$ into subintervals with a time step of $\Delta t = 0.5$. Figures 1 and 2 show the series solution of the MFTDM of the nonlinear fractional Riccati equations (15) and (16) for $\beta = 1, 0.7, 0.9$ and the exact. The graphical results show that the results produced using the MFTDM for $\beta = 1$ very closely correspond to the results of the exact solution. This emphasizes MFTDM applicability to many different kinds of nonlinear fractional differential equations, as well as its reliability and promise when compared to existing methods. Furthermore, as in the preceding instance, the numerical results produced by the MFTDM have the same course for various values of β . All results are obtained using Maple 16.

Example 2. Consider the following nonlinear fractional Riccati equation

$$D_*^\beta y(t) = 1 + 2y(t) - y^2(t), \quad t \geq 0, \quad 0 < \beta \leq 1, \tag{26}$$

with the initial condition

$$y(0) = 0. \tag{27}$$

The exact solutions of this equation when $\beta = 1$ is $y(t) = 1 + \sqrt{2} \tanh\left(\sqrt{2}t + \frac{1}{2} \log\left(\frac{\sqrt{2}-1}{\sqrt{2}+1}\right)\right)$. If $y_j(t)$ is an approximation in each subinterval $[t_{i-1}, t_i]$, $j = 1, 2, \dots, i$, the equations (26) and (27) can be transformed into the following system:

$$D_*^\beta y_j(t) = 1 + 2y_j(t) - y_j^2(t), \quad j = 1, 2, \dots, i. \tag{28}$$

$$y_j(t^*) = c_j, \tag{29}$$

With initial conditions with $c_1 = 1$.

Using the formable integral (denoted by F in this study) on both sides of Equation (28), we obtain

$$F \left[D_*^\alpha y_j(t) \right] = F \left[1 + 2y_j(t) - y_j^2(t) \right], \quad (30)$$

Equation (30) can be read using Theorem 2.3 and the initial condition in equation (29) as

$$F \left[y_j(t) \right] = c_j + \left(\frac{u}{s} \right)^\beta F \left[1 + 2y_j(t) - y_j^2(t) \right]. \quad (31)$$

Using the formable inverse on both sides of Equation (31) yields

$$\begin{aligned} y_j(t) = & F^{-1} \left[c_j \right] \\ & + F^{-1} \left[\left(\frac{u}{s} \right)^\beta F \left[1 + 2y_j(t) \right] \right] \\ & - F^{-1} \left[\left(\frac{u}{s} \right)^\beta f \left[y_j^2(t) \right] \right] \end{aligned} \quad (32)$$

Where $L \left[y_j(t) \right] = y_j(t)$, $N \left[y_j(t) \right] = y_j^2(t)$ are linear and nonlinear operators, respectively. The nonlinear term of Eq.(32) can be decomposed as

$$N \left[y_j(t) \right] = y_j^2(t) = \sum_{i=0}^{\infty} A_{j,i}. \quad (33)$$

Adomian polynomials' first few components are provided by

$$A_{j,0} = y_{j,0}^2,$$

$$A_{j,1} = 2y_{j,0}y_{j,1},$$

$$A_{j,2} = 2y_{j,0}y_{j,2} + y_{j,1}^2.$$

⋮

Assume that the solution of Equation (28) has the following series

$$y_j(t) = \sum_{i=0}^n y_{j,i}(t). \quad (34)$$

Substituting Equations (33) and (34) into Equation (32) yields

$$\sum_{i=0}^n y_{j,i}(t) = c_j + \quad (35)$$

$$F^{-1} \left[\left(\frac{u}{s} \right)^\beta F \left[1 + 2y_{j,i} - \sum_{i=0}^{\infty} A_{j,i} \right] \right].$$

After considering the comparison in Equation (35), we obtain

$$y_{j,0}(t) = c_j,$$

$$\begin{aligned} y_{j,1}(t) = & F^{-1} \left[\left(\frac{u}{s} \right)^\beta F \left[1 + 2y_{j,0} - A_{j,0} \right] \right] \\ = & \frac{(1 + 2c_j - c_j^2)(t - t^*)^\beta}{\Gamma(\beta + 1)}, \end{aligned}$$

$$\begin{aligned}
 y_{j,2}(t) &= F^{-1} \left[\left(\frac{u}{s} \right)^\beta F \left[2 y_{j,1} - A_{j,1} \right] \right] \\
 &= \frac{2 (1 - c_j) (1 + 2c_j - c_j^2) (t - t^*)^{2\beta}}{\Gamma(2\beta + 1)} \\
 &\quad - \frac{(1 + 2c_j - c_j^2)^2 \Gamma(2\beta + 1) (t - t^*)^{2\beta}}{\Gamma^2(\beta + 1) \Gamma(2\beta + 1)}, \\
 &\quad \vdots
 \end{aligned} \tag{36}$$

The series solution to equation (28) is provided by

$$\begin{aligned}
 y_j(t) &= c_j + \frac{(1 + 2c_j - c_j^2) (t - t^*)^\beta}{\Gamma(\beta + 1)} \\
 &\quad + \frac{2 (1 - c_j) (1 + 2c_j - c_j^2) (t - t^*)^{2\beta}}{\Gamma(2\beta + 1)} \\
 &\quad - \frac{(1 + 2c_j - c_j^2)^2 \Gamma(2\alpha + 1) (t - t^*)^{2\beta}}{\Gamma^2(\beta + 1) \Gamma(2\beta + 1)} + \dots
 \end{aligned}$$

In this example, the suggested method is applied to the interval $[0, 10]$. We selected dividing the interval $[0, 5]$ into subintervals with a time step of $\Delta t = 0.1$. Figures 3 and 4 show the series solution of the MFTDM of the nonlinear fractional Riccati equations (26) and (27) for $\beta = 1, 0.7, 0.9$ and the exact. The graphical results show that the results produced using the MFTDM for $\beta = 1$ very closely correspond to the results of the exact solution. This emphasizes MFTDM applicability to many different kinds of nonlinear fractional differential equations, as well as its reliability and promise when compared to existing methods. Furthermore, as in the preceding instance, the numerical results produced by the MFTDM have the same course for various values of β . All results are obtained using Maple 16.

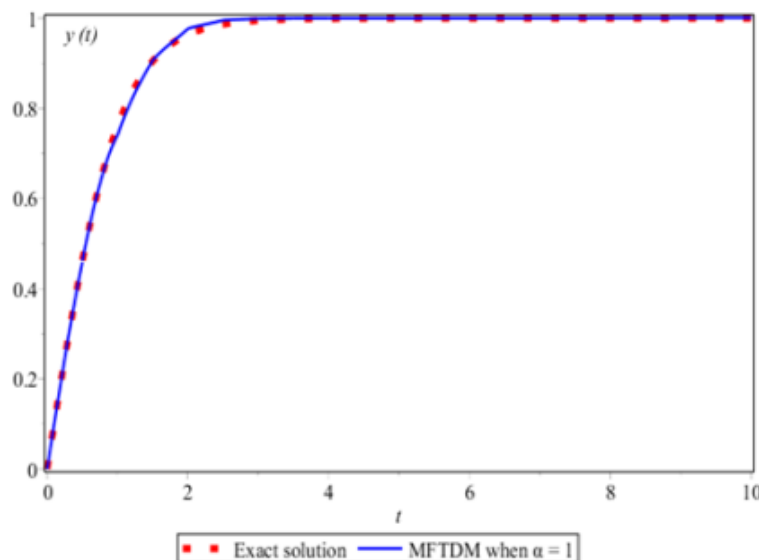


Figure: (1). Comparison between the exact and the MFTDM solutions of $y(t)$ for $\beta = 1$.

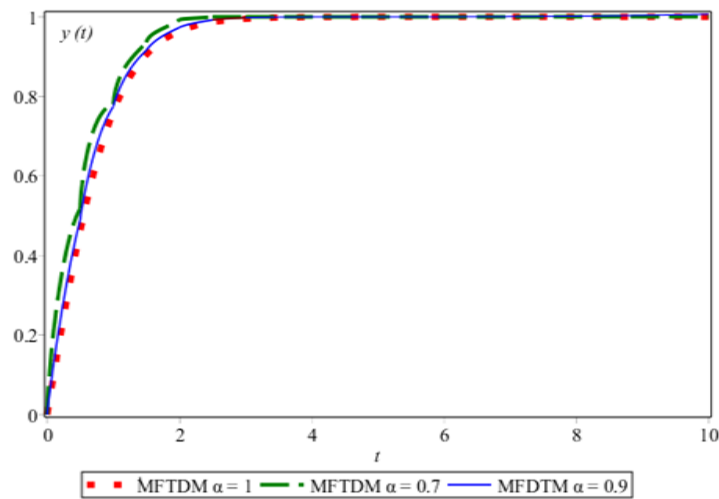


Figure: (2). The MFTDM solution of $y(t)$ for different values of β .

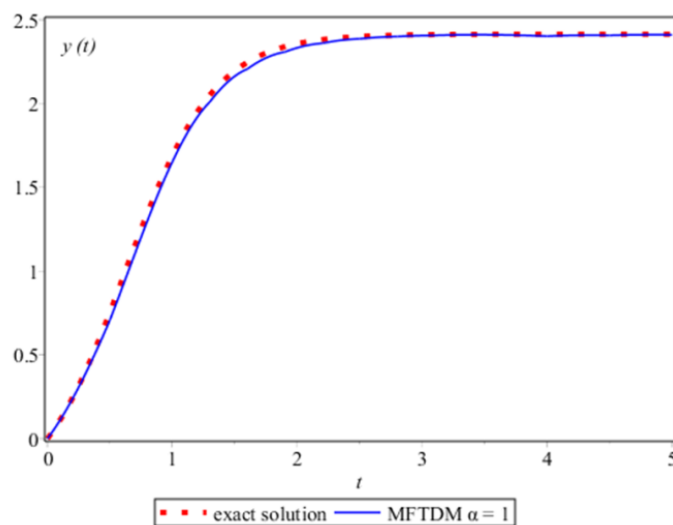


Figure: (3). Comparison between the exact and the MFTDM solutions of $y(t)$ for $\beta = 1$.

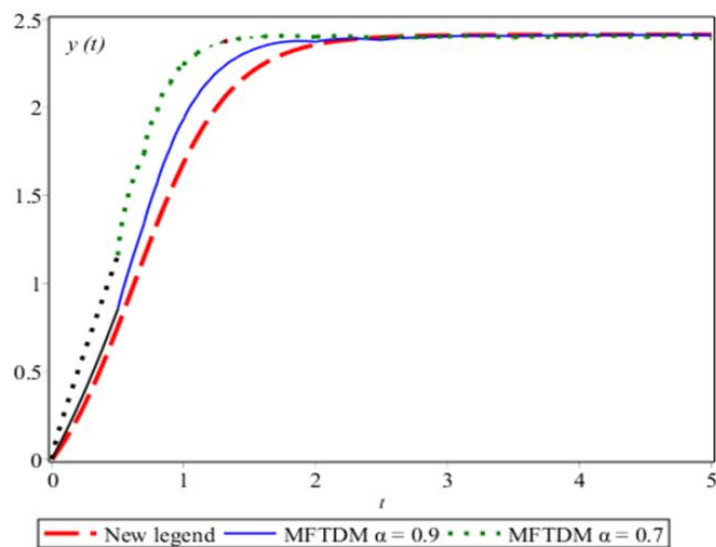


Figure: (4). The MFTDM solution of $y(t)$ for different values of β .

DISCUSSION

The graphical results show that the results produced using the MFTDM $\beta = 1$ very closely correspond to the results of the exact solution. This emphasizes the MFTDM applicability to many different kinds of nonlinear fractional differential equations, as well as its reliability and promise when compared to existing methods. Furthermore, as in the preceding instance, the numerical results produced by the MFTDM have the same course for various values of β . This is completely consistent with the research results of Al-Zoubi&Zurigat (2014).

CONCLUSION

A multi-step formable transform decomposition method (MFTDM) is suggested in this study to solve the nonlinear fractional-order Riccati problem. The MFTDM has been shown to solve fractional Riccati equations effectively, easily, and accurately. Approximate solutions quickly converge on exact solutions. This is completely consistent with the research results of Al-Zoubi&Zurigat (2014). Finally, we conclude that MFTDM is an excellent enhancement of existing numerical approaches. All results are obtained using Maple 16.

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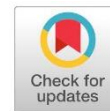
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Research Article

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On Strongly Regular Relation of Canonical Hypergroup

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Abstract

Burris and Sankappanavar established a connection between congruence in group G (ring R) and a normal subgroup of G (ideal of ring R). In this paper in the same manner, the connection between strongly regular relation defined on canonical hypergroup and normal subcanonical hypergroup of canonical hypergroup is established.

Keywords: canonical hypergroup, subcanonical hypergroup, normal subcanonical hypergroup, regular relation, strongly regular relation, and quotient of canonical hypergroup .

INTRODUCTION

The French mathematician Marty proposed the idea of hyperstructure, and particularly the idea of hypergroup, in 1934 (Marty, 1934). There are basic definitions and theories concerning the hyperstructures previously (AbouElwan & Alderawe, 2023; Davvaz *et al.*, 2023). Several fields of other disciplines can benefit from the use of hyperstructures. There have been numerous books and articles written about the use of hyperstructures in the study of geometry, hypergraphs, binary relations, lattices, fuzzy sets, etc (AbouElwan & Alderawe, 2023; Davvaz, 2012; Burris & Sankappanavar, 1981; Vougiouklis, 1994). Canonical hypergroup as a special kind of hypergroup is indeed a natural generalization of the concept of abelian group. This kind of hypergroup is a basic additive hyperstructure of many hyperstructures.

By applying a specific kind of equivalence relations, semihypergroup can be connected to semigroup, hypergroup to the group and canonical hypergroup to abelian group. These equivalence relations are called strongly regular relations. More exactly, by given (a semihypergroup, a hypergroup, and a canonical hypergroup) and by using a strongly regular relation on them, (a semigroup, a group, and the abelian group) respectively can be constructed from their quotient hyperstructures. (Corsini & Leoreanu, 2003)

MATERIALS AND METHODS

The definitions and examples from this section will be utilized throughout the paper.

A hyperoperation $\circ$ on a non-empty set H is a mapping $\circ: H \times H \rightarrow P^*(H)$, $P^*(H)$ is the power set of H , $\emptyset \notin P^*(H)$. Moreover, the pair $(H, \circ)$ is called a hyper-groupoid. For every A and $B \in P$



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$*(H)$ and $x \in H$, the sets $A \circ B$, $A \circ x$ and $x \circ A$ are defined by $A \circ B = \bigcup \{a \circ b \mid a \in A, b \in B\}$, $A \circ x = A \circ \{x\}$ and $x \circ A = \{x\} \circ A$.

A hypergroupoid $(H, \circ)$ is called a semihypergroup if for all a, b, c of H , we have $a \circ (b \circ c) = (a \circ b) \circ c$, this means that $\bigcup_{u \in b \circ c} a \circ u = \bigcup_{v \in a \circ b} v \circ c$. A semihypergroup $(H, \circ)$ is called a hypergroup if for every $a \in H$, we have $a \circ H = H \circ a = H$, that is called the reproduction axiom. A hypergroup $(H, \circ)$ is called a commutative hypergroup if for all $a, b \in H$, we have $a \circ b = b \circ a$. A non-empty subset K of a hypergroup $(H, \circ)$ is called a subhypergroup of H if K is a hypergroup under $\circ$. Several books have been written on hyperstructure theory (AbouElwan & Al-derawe, 2022; Velrajan & Asokkumar, 2010; Vougiouklis, 1994).

Let $(H, \circ)$ be a semihypergroup and R be an equivalence relation on H . If A, B are non-empty subsets of H , then $A\bar{R}B$ means that

$$\forall a \in A, \exists b \in B \text{ such that } aRb, \text{ and } \forall b' \in B, \exists a' \in A \text{ such that } a'Rb'.$$

Furthermore, $A\bar{\bar{R}}B$ means that

$$\forall a \in A, \forall b \in B, \text{ we have } aRb.$$

In addition, the equivalence relation R on H is said to be:

- 1) Regular on the left (on the right) if $\forall x \in H$, from aRb , it follows that $(x \circ a)\bar{R}(x \circ b)$ ($((a \circ x)\bar{R}(b \circ x)$ respectively).
- 2) Strongly regular on the left (on the right) if $\forall x \in H$, from aRb , it follows that $(x \circ a)\bar{\bar{R}}(x \circ b)$ ($((a \circ x)\bar{\bar{R}}(b \circ x)$ respectively).
- 3) Strongly regular (Regular) if it is strongly regular (regular) on the right and on the left. (see 6).

Let $(H, \circ)$ be a hypergroup, for an equivalence relation R on H , we use $R(x)$ to denote the equivalence class of x to R and use H/R to denote the family of equivalence classes $\{R(x) \mid x \in H\}$ of R . The reader can find the proofs of the following two theorems in (BDavvaz & Leoreanu-Fotea, 2007; Davvaz *et al.*, 2022).

Theorem 2.1. If $(H, \circ)$ is a hypergroup (a semihypergroup) and R is a regular relation on H , then the quotient H/R is a hypergroup (a semihypergroup) under the operation defined by

$$R(x) \otimes R(y) = \{R(z) \mid z \in x \circ y\}.$$

Theorem 2.2. If $(H, \circ)$ is a hypergroup (a semihypergroup) and R is a strongly regular relation on H , then the quotient H/R is a group (a semigroup) under the operation defined by

$$R(x) \otimes R(y) = R(z), \forall z \in x \circ y.$$

Definition 2.3. A canonical hypergroup $(M, +)$ is a non-empty set M together with a hyperoperation $+$ which satisfies the following axioms:

- i. $\forall x, y \in M, x + y = y + x$,
- ii. $\forall x, y, z \in M, x + (y + z) = (x + y) + z$,
- iii. $\exists 0 \in M$ (called neutral element of M) such that

$$0 + x = \{x\} = x + 0, \forall x \in M,$$

- iv. $\forall x \in M, \exists_1 -x \in M$ such that

$$0 \in x + (-x) \cap (-x) + x,$$

v. the reversibility axiom:

$$\forall x, y, z \in M, z \in x + y \Rightarrow y \in -x + z \text{ and } x \in z + (-y).$$

Let $(M, +)$ be a canonical hypergroup, a non-empty subset N of $(M, +)$ is called a subcanonical hypergroup of M if $(N, +)$ is a canonical hypergroup itself. Equivalently, $x - y \subseteq N, \forall x, y \in N$.

In particular, $\forall x \in N, x - x \subseteq N$. Since $0 \in x - x$, it follows that $0 \in N$. Moreover, N is said to be normal if $x + N - x \subseteq N$, for all $x \in M$. In addition, a subcanonical hypergroup N of M is called a subgroup of M if $(N, +)$ is a group, that is, if $x + y$ is a singleton set for all $x, y \in N$.

Example 2.4. Consider the set $M = \{0, a, b\}$. Define a hyperaddition $+$ on M as in the following table

$+$	0	A	b	c
0	$\{0\}$	$\{a\}$	$\{b\}$	$\{c\}$
a	$\{a\}$	$\{0, b\}$	$\{a, c\}$	$\{b\}$
b	$\{b\}$	$\{a, c\}$	$\{0, b\}$	$\{a\}$
c	$\{c\}$	$\{b\}$	$\{a\}$	$\{0\}$

Then, $(M, +)$ is a canonical hypergroup, $\{0, b\}$ is a subcanonical hypergroup of M , and $\{0, c\}$ is a subgroup of M .

Remark 2.5. If N be a subcanonical hypergroup of a canonical hypergroup $(M, +)$, then the quotient is $M/N = \{x + N \mid x \in M\}$,

where $x + N = \{x + n \mid n \in N\}$, we will use $\bar{x}$ instead of $x + N$.

Theorem 2.6.^[11] If N be a subcanonical hypergroup of a canonical hypergroup $(M, +)$. Then M/N is a canonical hypergroup with respect to the following hyperoperation

$$(x + N) \oplus (y + N) = \{z + N \mid z \in x + y\}, \text{ for all } x + N, y + N \in M/N.$$

Proof. Let $x_1, y_1, x_2, y_2 \in M$ such that $\bar{x}_1 = \bar{x}_2$ and $\bar{y}_1 = \bar{y}_2$ then $x_2 \in x_1 + N$ and $y_2 \in y_1 + N$. Let $z_2 \in x_2 + y_2 \subseteq (x_1 + N) + (y_1 + N)$. Since M is commutative, $z_2 \in z_1 + n$ for some $z_1 \in x_1 + y_1$ and for some $n \in N$. That is, $z_2 + N = z_1 + N$. Hence,

$$\bar{x}_2 \oplus \bar{y}_2 \subseteq \bar{x}_1 \oplus \bar{y}_1.$$

Also, since $x_1 \in x_2 + N$ and $y_1 \in y_2 + N$, by a similar argument, we get,

$$\bar{x}_1 \oplus \bar{y}_1 \subseteq \bar{x}_2 \oplus \bar{y}_2.$$

Hence, $\bar{x}_1 \oplus \bar{y}_1 = \bar{x}_2 \oplus \bar{y}_2$. Thus, $\oplus$ is well defined.

Let $\bar{x}, \bar{y}, \bar{z} \in M/N$. If $\bar{u} \in (\bar{x} \oplus \bar{y}) \oplus \bar{z}$, then $\bar{u} \in \bar{p} \oplus \bar{z}$ for some $\bar{p} \in \bar{x} \oplus \bar{y}$. That is, $\bar{u} = \bar{a}$ for some $a \in p + z$. Also $\bar{p} = \bar{b}$ for some $b \in x + y$.

Now, $a \in p + z \subseteq b + N + z = b + z + N$. That is, $a \in v + N$ for some $v \in b + z \subseteq (x + y) + z = x + (y + z)$. So, $v \in x + t$ for some $t \in y + z$. This means that, $\bar{a} = \bar{v}$ and $\bar{v} \in \bar{x} \oplus \bar{t}$. Since $\bar{t} \in \bar{y} \oplus \bar{z}$, we have

$$\bar{u} = \bar{a} = \bar{v} \in \bar{x} \oplus \bar{t} \subseteq \bar{x} \oplus (\bar{y} \oplus \bar{z}).$$

This means that, $\bar{u} \in \bar{x} \oplus (\bar{y} \oplus \bar{z})$. Hence,

$$(\bar{x} \oplus \bar{y}) \oplus \bar{z} \subseteq \bar{x} \oplus (\bar{y} \oplus \bar{z}).$$

Similarly, we get

$$\bar{x} \oplus (\bar{y} \oplus \bar{z}) \subseteq (\bar{x} \oplus \bar{y}) \oplus \bar{z}. \text{ Hence, } (\bar{x} \oplus \bar{y}) \oplus \bar{z} = \bar{x} \oplus (\bar{y} \oplus \bar{z}).$$

Thus, the hyperoperation $\oplus$ is associative.

Consider the element $\bar{0} = 0 + N \in M/N$. Now, for any $x \in M$, we have

$$\bar{x} \oplus \bar{0} = \{\bar{z} \mid z \in x + 0\} = \bar{x}.$$

Similarly, $\bar{0} \oplus \bar{x} = \bar{x}$. Thus, $\bar{0}$ is the zero element of M/N .

Let $x \in M$, then $\bar{x} \oplus (-\bar{x}) = \{\bar{z} \mid z \in x + (-x) = x - x\}$. Since $\bar{0} \in x - x$, we get, $\bar{0} \in \bar{x} \oplus (-\bar{x})$. Similarly, $\bar{0} \in (-\bar{x}) \oplus \bar{x}$. Let $\bar{x} \in M/N$, and suppose that $\bar{y} \in M/N$ such that $\bar{0} \in \bar{y} \oplus \bar{x}$, then $\bar{0} = \bar{a}$, where $a \in y + x$. That is, $y \in a - x \subseteq N - x$, and hence $\bar{y} = -\bar{x}$. Thus, the element $\bar{x} \in M/N$ has a unique inverse $-\bar{x} \in M/N$. Suppose that $\bar{z} \in \bar{x} \oplus \bar{y}$, then $\bar{z} = \bar{a}$, where $a \in x + y$. This implies,

$x \in a - y \subseteq z + N - y$. That is, $x \in r + N$, where $r \in z - y$. Thus, $\bar{x} = \bar{r} \in \bar{z} \oplus (-\bar{y})$. Similarly, we can show that $\bar{y} \in (-\bar{x}) \oplus \bar{z}$. Since M is commutative, it is obvious that M/N is also commutative. Thus, M/N is a canonical hypergroup. ■

Theorem 2.7.^[11] Let $(M, +)$ be a canonical hypergroup, and let N be a normal subcanonical hypergroup of M . Then, $(M/N, \oplus)$ is an abelian group.

RESULTS

Definition 3.1. Let $(M, +)$ be a canonical hypergroup, and ρ be an equivalence relation on M , then ρ is called:

- 1) Regular if for all $a, b \in M$, apb implies that for every $x \in M$, for every $u \in a + x$ there exists $v \in b + x$ such that upv and for every $v' \in b + x$ there exists $u' \in a + x$ such that $u'pv'$.
- 2) Strongly regular if for all $a, b \in M$, apb implies that for every $x \in M$, for every $u \in a + x$ and for every $v \in b + x$ one has upv .

Proposition 3.2.^[6] Let $(M, +)$ is a canonical hypergroup, and let N be a normal subcanonical hypergroup of M . Then, for all $x, y \in N$, the following are equivalent:

- i. $y \in x + N$,
- ii. $x - y \subseteq N$,
- iii. $(x - y) \cap N \neq \emptyset$.

Proof.

(i $\Rightarrow$ ii). Since $y \in x + N$, we have $y - x \subseteq x + N - x$, and since N is normal subcanonical hypergroup of M , we get $x + N - x \subseteq N$. Thus, $y - x \subseteq N$. That is, $-(y - x) \subseteq N$, and hence $x - y \subseteq N$.

(ii $\Rightarrow$ iii). Is obvious.

(iii $\Rightarrow$ i). Since $(x - y) \cap N \neq \emptyset$, there exists $a \in x - y$ and $a \in N$. Therefore, $-y + x \subseteq -y + a + y \subseteq N$. If $z \in -y + x$, then $z \in N$. Therefore, $-y \in z - x$. That is, $y \in x - z \subseteq x + N$. ■

Now, if $(M, +)$ is a canonical hypergroup, then we can establish the following connection between regular relations on M and subcanonical hypergroups of M , and establish a similar connection between strongly regular relations on M and normal sub-canonical hypergroups of M as follows:

i. If ρ is a regular relation on M . Then the equivalence class $\rho(0)$ is a subcanonical hypergroup of M , where 0 is a neutral element of M . For $a, b \in M$, we have

$$apb \text{ iff } a \in b + \rho(0).$$

ii. If ρ is a strongly regular relation on M . Then the equivalence class $\rho(0)$ is a normal subcanonical hypergroup of M , where 0 is a neutral element of M . For $a, b \in M$, we have

$$apb \text{ iff } a - b \subseteq \rho(0).$$

Theorem 3.3. Let $(M, +)$ be a canonical hypergroup, and let N be a normal subcanonical hypergroup of M . If a, b are elements in M , then the binary relation ρ defined on M by:

$$apb \text{ iff } a - b \subseteq N,$$

is a strongly regular on M with $\rho(0) = N$.

Proof. Let $a, b, c \in M$. Clearly, $a \in a + 0$, implies

$$a - a \subseteq a + 0 - a \subseteq a + N - a \subseteq N.$$

So ρ is reflexive. Also, $a - b \subseteq N$ if and only if $b - a \subseteq N$. So ρ is symmetric. For transitivity, if $a - b \subseteq N$ and $b - c \subseteq N$ then by normality of N , we have

$$a - b + b - c = a - b + 0 + b - c \subseteq a + N - c \subseteq a - c + N \subseteq N,$$

$$a - c \subseteq N.$$

Thus ρ is an equivalence relation on M .

Next, to prove that the equivalence relation ρ is a strongly regular on M , suppose that apb then $a - b \subseteq N$, let $x \in M$, if $u \in a + x$ and $v \in b + x$, then

$u - v \subseteq a + x - (b + x) = a + x - (x + b) = a + (x - x) - b \subseteq a + (x + 0 - x) - b \subseteq a + N - b \subseteq N$, so upv , thus

$$(a + x)\bar{\rho}(b + x).$$

Hence ρ is a strongly regular relation on M .

Now, to prove that $\rho(0)$ is a normal subcanonical hypergroup of M . Let $a, b \in \rho(0)$, then $ap0$ and $b\rho0$, since ρ is a strongly regular relation on M . this imply that

$$(a + b)\bar{\rho}(0 + 0),$$

this means that, for all $u \in a + b$ and $0 \in 0 + 0$, we have $u\rho0$, it follows that

$$u \in \rho(0), \text{ so } a + b \subseteq \rho(0).$$

Since $a \in \rho(0)$ it follows that $-a \in \rho(0)$. Therefore $\rho(0)$ is a subcanonical hypergroup of M . For normality of $\rho(0)$, let $a \in \rho(0)$ and $x \in M$, then

$$(x + a)\bar{\rho}(x + 0),$$

this implies that $(x + a)\bar{\rho}x$,

it follows that $(x + a - x)\bar{\rho}(x - x)$,

then $(x + a - x)\bar{\rho}0$, since $0 \in x - x$.

Therefore, $x + a - x \subseteq \rho(0)$.

Thus $\rho(0)$ is a normal subcanonical hypergroup of M .

Finally, to prove that $\rho(0) = N$, if $a \in \rho(0)$ then $a\rho 0$ implies $a - 0 \subseteq N$, so $a \in N$, thus $\rho(0) \subseteq N$. Conversely, if $a \in N$ then $a - 0 \subseteq N$, it follows that $a\rho 0$ implies $a \in \rho(0)$, thus $N \subseteq \rho(0)$. Hence, $\rho(0) = N$. ■

CONCLUSION

By strongly regular relation defined on a canonical hypergroup M , the equivalence class $\rho(0)$ is exactly a normal subcanonical hypergroup of M .

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

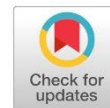
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Approximate confidence intervals for the Population Proportion based on linear model



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Abstract

When the linear model errors are non-normal, one might be interested in making inferences concerning proportion. The goal of this article is to construct approximate confidence intervals for the proportion founded on the supposed linear model which covers a true value of a proportion that is close to a specific nominal value of the level of significant.

Keywords: Linear model, central limit theorem, slusky's lemma, asymptotic distribution, confidence intervals.

INTRODUCTION

In this paper study was derived the asymptotic confidence intervals by the z-quantile and by the t-quantile, to construct approximate confidence intervals of the proportion based on linear models.

Then it was introduced to the used model:

suppose that the sum random variable X_i is a Poisson distribution can be splits into two separate Poisson random variables Y_i, Z_i with means λ_1, λ_2 respectively. It means.,

$X_i \sim (\lambda_1, \lambda_2)$, and since $E(Y_i) = \text{Var}(Y_i) = \lambda_1$, and $E(Z_i) = \text{Var}(Z_i) = \lambda_2$, consequently

$E(X_i) = \text{Var}(X_i) = \lambda_1 + \lambda_2$. Further,

$P(Y_i | X_i) \sim \text{Bin}(X, p)$, where $p = \frac{\lambda_1}{\lambda_1 + \lambda_2}$, $X_i > 0$ ($\text{B}(n, p)$ denotes the

Binomial distribution with parameters n, p).

The remainder of the paper was organized as follows: Description of the assumed model is given in Sec 2. Estimation of linear model parameter were given in Sec. 3. Section 4 to provide confidence intervals for the proportion.

The Linear model

Suppose, there are m observations of two relevant components of data, i.e., $(Y_i, X_i); i = 1, \dots, m$ are $m \times 2$ dimensional observed data since every observational item referenced by the subscript i , as well as, $Y_i, X_i > 0; \forall i = 1, \dots, m$. The i^{th} observation represents unit, for example:

$X_i \equiv$ number of units for a product $i; i = 1, \dots, m$



$Y_i \equiv$ number of damaged units for a product i ; $i = 1, \dots, m$.

Consider the univariate linear model $Y_i = x_i p + \epsilon_i$, $i = 1, \dots, m$, with the following assumptions:

$E(Y_i) = x_i p$, $E(\epsilon_i) = 0$, also by variance relational to x_i (x_i is fixed variable), i.e.,
 $Var(Y_i) = Var(\epsilon_i) = \sigma^2 x_i$, compressing the model in vector form (for the i^{th} observation) yields:
 $Y_i = Xp + \epsilon$, ($i = 1, \dots, m$), where

$Y = (Y_1, \dots, Y_m)^T$, and the $m \times 1$ design vector.

$X = (x_1, \dots, x_m)^T$, then the heteroscedastic errors $(\epsilon_1, \dots, \epsilon_m)^T = \epsilon$, through the expectations,
 $E(\epsilon) = \mathbf{0}_m$, and $Var(\epsilon) = \sigma^2 W$, where $\mathbf{0}_m = (0, \dots, 0)^T$, and $W = \text{diag}(x_i)$. The single model was weighted by the linear transformation

$$A_i Y_i = A_i x_i p + A_i \epsilon_i,$$

$$\tilde{Y}_i = \tilde{x}_i p + \tilde{\epsilon}_i, i = 1, \dots, m \quad [2.1]$$

where, $A_i = \frac{1}{\sqrt{x_i}}$, given that $x_i > 0$, $\tilde{Y}_i = A_i Y_i = \frac{Y_i}{\sqrt{x_i}}$, $\tilde{x}_i = A_i x_i = \sqrt{x_i}$, $\tilde{\epsilon}_i = A_i \epsilon_i = \frac{\epsilon_i}{\sqrt{x_i}}$, it follows that
 $E(\tilde{\epsilon}_i) = 0$, and $Var(\tilde{\epsilon}_i) = \sigma^2$, $\forall i = 1, \dots, m$ (homoscedastic errors), as well as
 $Cov(\epsilon) = \sigma^2 I_m = Cov(\tilde{Y})$. such that I_m is an Identity Matrix of elements $m \times m$, also the weighted response vector $\tilde{Y} = (\tilde{Y}_1, \dots, \tilde{Y}_m)^T$, and the weighted design vector $\tilde{X} = (\tilde{x}_1, \dots, \tilde{x}_m)^T$, as well as the weighted error vector $\tilde{\epsilon} = (\tilde{\epsilon}_1, \dots, \tilde{\epsilon}_m)^T$, where

$$\sigma^2 = E(\tilde{Y}_i - \tilde{X}_i p)^2$$

Estimation in linear models

Agreeing whether the demonstrate blunders are homoscedastic or heteroscedastic blunders we estimate the proportion p .

Heteroscedasticity

Since, error of the vector of the non-weighted ideal has covariance that is the variance proportional to the known invertible diagonal matrix W ; so, it is the Generalized Least Squares Estimator, that is further the Best linear unbiased estimator. The covariance structure is given by

$$\text{cov}(\epsilon) = \begin{bmatrix} \sigma^2 x_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma^2 x_m \end{bmatrix} = \sigma^2 W$$

x_i are fixed, $i = 1, \dots, m$ and $W^{-1}W = I_m$, as well as $X^T W = 1_m^T$, where $1_m = (1, \dots, 1)^T$. So, we have

$$\hat{p}_{GLS} = (X^T (\sigma^2 W)^{-1} X)^{-1} X^T (\sigma^2 W)^{-1} Y = (X^T W^{-1} X)^{-1} X^T W^{-1} Y$$

Homoscedasticity

It is familiar and defined very well; that the Weighted Least Squares Estimator is the Best linear unbiased estimator, in addition, due to the reason that, the weighted errors are homoscedastic therefore, the Weighted Least Squares Estimator functional to the Model 2.1 concludes in the OLS Estimator, hence is also the greatest LUE, according to Gauss-Markov's theorem (1-3), i.e., $\hat{p}_{WLS} = \hat{p}$. Since, $\text{cov}(\tilde{\epsilon}) = \sigma^2 I_m$,

then

$$\begin{aligned}\hat{p}_{WLS} &= (\tilde{X}^T (\sigma^2 I_m)^{-1} \tilde{X})^{-1} \tilde{X}^T (\sigma^2 I_m)^{-1} \tilde{Y} = (X^T I_m X)^{-1} \tilde{X}^T I_m \tilde{Y} \\ &= \left(\sum_{i=1}^m (\sqrt{x_i})^2 \right)^{-1} \sum_{i=1}^m \sqrt{x_i} \tilde{Y}_i = \frac{\sum_{i=1}^m \sqrt{x_i} \tilde{Y}_i}{\sum_{i=1}^m x_i} = \frac{\sum_{i=1}^m Y_i}{\sum_{i=1}^m x_i} = \hat{p}, \\ &\quad \sqrt{x_i} \tilde{Y}_i = Y_i.\end{aligned}$$

Asymptotic normal for the ratio $\hat{p}_m$

It supposed that the random errors $\tilde{\epsilon}_i$ are not Normally Distributed nonetheless are independently identical distributed random variables, $i = 1, \dots, m$, i.e., $E(\tilde{\epsilon}_i) = 0$, and $\text{Var}(\tilde{\epsilon}_i) = 0$. Furthermore, under a positive conditions on the project X we can demonstrate that in huge sample sizes, $\hat{p}$ obeys the asymptotic normal distribution.

And more additionally conditions on the couple of observations X_i, Y_i are required, called (X_i, Y_i) are independently identical distributed pairs of random variables, plus $E(X_i)$ exist $\Rightarrow$

$(\tilde{X}_i, \tilde{Y}_i)$ are then independently identical distributed random variables, furthermore $E(\tilde{X}_i^2)$ exists

$$i = 1, \dots, m, \tilde{X}_i = \sqrt{X_i}, \tilde{Y}_i = \frac{Y_i}{\sqrt{x_i}}, X_i > 0.$$

To arrive to the asymptotic distribution, one rephrases first the estimator $\hat{p}_m$ as

$$\begin{aligned}\hat{p}_m &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{Y} = \left(\sum_{i=1}^m \tilde{X}_i \tilde{X}_i \right)^{-1} \sum_{i=1}^m \tilde{X}_i \tilde{Y}_i \\ &= \left(\sum_{i=1}^m X_i \right)^{-1} \sum_{i=1}^m \tilde{X}_i (\tilde{X}_i p + \tilde{\epsilon}_i) = \left(\sum_{i=1}^m X_i \right)^{-1} \left(\sum_{i=1}^m \tilde{X}_i p + \sum_{i=1}^m \tilde{X}_i \tilde{\epsilon}_i \right) \\ &= p + \left(\sum_{i=1}^m X_i \right)^{-1} \sum_{i=1}^m \tilde{X}_i \tilde{\epsilon}_i\end{aligned}\quad (3.1)$$

Consequently

$$\sqrt{m}(\hat{p}_m - p) = \left(\frac{1}{m} \sum_{i=1}^m X_i \right)^{-1} \frac{1}{\sqrt{m}} \left(\sum_{i=1}^m \sqrt{\tilde{X}_i} \tilde{\epsilon}_i \right) = \left(\frac{1}{m} \sum_{i=1}^m X_i \right)^{-1} \frac{1}{\sqrt{m}} \left(\sum_{i=1}^m \sqrt{X_i} \tilde{\epsilon}_i \right) \quad (3.2)$$

The asymptotic of the equation 3.2, requests to confirm, the denominator in 3.2 is reliable, and the numerator submits the CLT. It direct to see (by the LLN)

$$= \left(\frac{1}{m} \sum_{i=1}^m X_i \right)^{-1} \xrightarrow{p} (E(X_i))^{-1},$$

Given that, $E(X_i) > 0$, and

$$= \left(\frac{1}{m} \sum_{i=1}^m x_i \right)^{-1} \rightarrow \mu^{-1}, \quad \mu \text{ is a constant.}$$

Along with the numerator

$\frac{1}{\sqrt{m}} \sum_{i=1}^m \sqrt{X_i} \tilde{\epsilon}_i \xrightarrow{D} N(0, \sigma^2 E(X_i))$, where, the marginal or asymptotic variance

$$\begin{aligned} \text{cov}(\sqrt{X_i} \tilde{\epsilon}_i, \sqrt{X_i} \tilde{\epsilon}_i) &= \text{Var}(\sqrt{X_i} \tilde{\epsilon}_i) = E(X_i \text{Var}(\tilde{\epsilon}_i \setminus \tilde{X}_i)) + \text{Var}(E(\sqrt{X_i} \tilde{\epsilon}_i \setminus \tilde{X}_i)) \\ &= \sigma^2 E(X_i). \end{aligned}$$

As a result, following the use of the Slutsky's lemma (see [Knight,. 2000], pp. 119-120), the equation 3.2 can be rewritten as

$$\sqrt{m}(\hat{p}_m - p) \xrightarrow{D} N(0, \sigma^2 E(X_i)(E(X_i))^{-2}) \equiv N(0, \sigma^2 (E(X_i))^{-1}) \quad (3.3)$$

Approximate Confidence Intervals for the Population Proportion p

From 3.3, the asymptotic variance,

$$\text{Var}(\sqrt{m}(\hat{p}_m)) = E(\text{Var} \sqrt{m}(\hat{p}_m) \setminus \mathbf{X}^T) + \text{Var}(E \sqrt{m}(\hat{p}_m) \setminus \mathbf{X}^T) = \frac{\sigma^2}{E(X_i)},$$

$$\text{as } \text{Var}(E \sqrt{m}(\hat{p}_m) \setminus \mathbf{X}^T) = 0, \mathbf{X} = (X_1, X_2, \dots, X_m)^T.$$

conclude that , the estimated $(1 - \alpha)\%$ asymptotic confidence interval for the amount p is given by

$\left[\hat{p}_m \pm z_{1-\frac{\alpha}{2}} s.e(\hat{p}_m) \right]$, where, the standard error of $\hat{p}_m$

$$, s.e(\hat{p}_m) = \frac{s_m}{\sum_{i=1}^m X_i}, \quad s_m^2 = \frac{1}{m-1} \sum_{i=1}^m (Y_i - \hat{p} \tilde{X}_i)^2.$$

Further and since $\bar{X}_m$ and s_m^2 are consistent estimators for $E(X_i)$ and σ^2 respectively, it follows that consistent estimator of the $\text{Var}(\hat{p}_m)$ is $\frac{s_m^2}{\sum_{i=1}^m X_i}$ similarly, such as

$$\frac{\hat{p}_m - p}{\frac{s_m^2}{\sum_{i=1}^m X_i}} \sim t_{m-1} \xrightarrow{D} N(0,1)$$

Henceforth, the interval that is safety bounds provided by

$$\left[\hat{p}_m \pm t_{(m-1, 1-\frac{\alpha}{2})} s.e(\hat{p}_m) \right],$$

is the recommended more conservative confidence interval for p , where $s.e(\hat{p}_m) = \frac{s_m}{\sum_{i=1}^m X_i}$, as well as $t_{(m-1, 1-\frac{\alpha}{2})}$ is $(1 - \frac{\alpha}{2})$ percentile of the student t distribution with $(m - 1)$ degrees of freedom.

CONCLUSION

Results obtained from this article two confidence intervals first is the asymptotic confidence interval and the second is the extra conservative asymptotic confidence interval for the population proportion which can give more reliable intervals to cover the true population proportion P . Hence we considered two confidence intervals, the asymptotic (following the normal quintile) in addition the proposed conservative (with the adjusted t-quintile) confidence intervals.

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript..

Author contributions: The author did all the work related to the manuscript, including designing the research, collecting information, formulating theories and proofs, and preparing the entire paper.

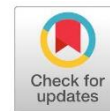
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Research Article

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Hybrid Dual Quadrature Rules Combining Open and Closed Quadrature Rules Enhanced by Kronrod Extension or Richardson's Extrapolation for Numerical Integration

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Abstract

Numerical integration is a powerful way to integrate certain categories of integrals, such as those whose closed-form anti-derivative is absent, improper integrals, and tabular data where a function is absent. In this paper, open and closed dual hybrid quadrature rules have been designed for the numerical integration of real definite integrals with either a singular integrand or a non-elementary anti-derivative, respectively. Such quadrature rules couple a Gauss-type rule with a Newton-Cotes-type rule such that both rules are of the same degree of precision, say p to achieve a hybrid rule of a degree of precision greater than or equal to $p+2$. The open/closed-type hybrid quadrature rule has been constructed as a linear combination between the two-point Gauss-Legendre quadrature enhanced by Kronrod extension and a derivative-based open/closed Newton-Cotes formula yielding a hybrid rule of degree of precision equal to nine. Furthermore, a hybrid quadrature rule was created by merging the numerically enhanced Lobatto-Gauss rule and Bool's rule which was enhanced by Richardson extrapolation. An error analysis analytically confirms that the proposed rules perform better than their ingredients' quadrature rules. The effectiveness of the suggested hybrid rules has been demonstrated with some integral examples that exhibit good agreement with the near-exact results. An adaptive quadrature rule has been implemented to considerably enhance the results' accuracy.

Keywords: Gaussian Quadrature, Bool's Rule, Kronrod Extension, Richardson Extrapolation, Hybrid Quadrature Rule, Derivative-Based Open & Closed Newton-Cotes Quadrature Formulae, Mixed Quadrature Rule, Numerical Quadrature.

INTRODUCTION

Numerical integration is a widespread technique to integrate specific categories of integrals with some restrictions, such as integrals that do not possess a closed form, elementary anti-derivatives, or improper integrals. One of the very popular tools for numerical integration is the quadrature rules, either Gauss-type or Newton-Cotes-type (Atkinson, 2012; Davis and Rabinowitz, 2012; Burden and Faires, 2005). Quadrature rules are commonly implemented in a variety of applications in physics, engineering, and quantum mechanics. Such quadrature rules are very convenient for computing the anti-derivative of tabular data, which may be encountered in some applications from experiments or measurements where the function is absent. Gauss-type and Newton-Cotes-



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type quadrature rules are both open, closed, and semi-open types; this should increase their reliability in adopting a variety of integrals with certain constraints. Numerical integration can efficiently integrate improper integrals of different types. Improper integrals over the infinite intervals $(0, \infty)$ or $(-\infty, \infty)$ can be efficiently integrated by Gauss-Lagurre or Gauss-Hermite, respectively (Das and Dash, 2017). Furthermore, such improper integrals can be transformed by a suitable transformation yielding finite limits of integration, then recall a convenient rule for the finite intervals. Gaussian quadrature rules are widely used for integral oscillatory or singular integrands that are encountered in many applications, as evidenced by (Milovanovic, 1998). A comparison between Newton-Cotes quadrature rules and Gaussian quadrature rules is presented in (Sermutlu, 2005) in terms of accuracy, computational effort, and number of integrand evaluations. He claimed that by using low and high-order rules, the quadrature rules of Gauss-Type are superior to the standard Newton-Cotes-Type rules.

The degree of precision of quadrature rules can be improved either by increasing the number of nodes n or decreasing the step size h . However, this may adversely affect the stability of the numerical rule due to the undesirable appearance of negative weights which leads to an ill-conditioned numerical process. Thus, one could resort to the adaptive scheme either globally (on the whole interval of integration) if needed or locally along some sub-regions where the integrand has sharp variation. The mechanism of the adaptive technique is to densely evaluate the integrand in certain sub-intervals where the function experiences large variation to capture the behavior of the integrand in such regions until the termination criterion is met (Dash and Das, 2013a; Dash and Das, 2013b; Dash and Das, 2012). A new set of closed, Mid-point, and open Newton-Cotes quadrature rules were proposed by Burg et. al. (Burg, 2012; Burg, 2013; Zafar, 2014). Such new derivative-based Newton-Cotes formulae require the evaluations of the integrand and its derivative at less abscissa compared to the classical Newton-Cotes rules. They claim that the new scheme of Newton-Cotes formulae yields much better performance compared with the standard Newton-Cotes formulae in terms of accuracy, computational effort, arithmetic operations of the integrand, degree of precision, error terms, and their coefficients.

The degree of precision of n -point the Gaussian rule is $(2n - 1)$, that is this rule should exactly integrate any polynomials of a degree less than or equal to $(2n - 1)$. The n -point Newton-Cotes quadrature rules are of the degree of precision $(n - 1)$ if n is even, and of the degree of precision n if n is odd. Recently, a numerical enhancement was proposed by (Babolian et al., 2005; Masjed et. al., 2005) to increase the accuracy by two for the Gauss-Legendre and Gauss-Radau quadrature rules. Furthermore, a numerical enhancement of the Gauss-Lobatto quadrature rule was proposed by (Eslahchi et. al., 2005), and they claim that they obtained better approximate results than those obtained by the corresponding standard Gauss-Lobatto quadrature rule. Moreover, such a technique has been adopted for the open, closed, and semi-open Newton-Cotes formulae, respectively (Dehghan et. al., 2006; Dehghan et. al., 2005a; Dehghan et. al., 2005b).

It is worth emphasizing that those Gaussian quadrature rules are stable because all the weights are positive. Gauss-Legendre, Hermite, and Lagurre quadrature rules are of open type, whereas Gauss-Lobatto and right/left Gauss-Radaua are respectively of closed and semi-open/closed type. A drawback of Gauss-type rules is that they are not progressive, that is, Gaussian rules of differentiation, and have no nodes in common except at the midpoint. To overcome the non-progressive issue related to Gaussian quadrature rules, Kronrod (Kronrod, 1965 a; Kronrod, 1965 b; Walter, 1988) established his extension to the Gauss-Legendre and Lobatto quadrature rules, both of which have a weight function ($w(x) = 1$). The Kronrod extension optimally adds $(n + 1)$ abscissas to the n -point Gaussian, yielding a more accurate $(2n + 1)$ -point Kronrod–Legendre Gauss pair quadrature rule.

In contrast, for other Gaussian quadrature rules, such as Hermite-Gauss and Laguerre-Gauss, there is no real Kronrod extension (Kahaner, 1978), but sub-optimal Kronrod extensions can be gained with a degree of precision less than $(3n + 1)$ (Begumisa and Robinson, 1991). Additionally, Patterson (Patterson, 1968 a; Patterson, 1968 b) enlarged the idea of Kronrod extension by adding $(2n + 2)$ points to the $(2n + 1)$ -point Kronrod–Gauss pair to achieve a progressive rule of $(6n + 4)$ as a degree of precision.

The accuracy of the numerical quadrature rules can be enhanced by adopting some reliable approaches such as Richardson's extrapolation (Burden and Faires 2005) and the Kronrod extension which respectively rely on the trapezoidal rule and quadrature rule as a fundamental rule. Richardson extrapolation (Zlatev et. al., 2018) is a powerful technique to enhance the accuracy of approximation numerical tools that deal with a parameter say the step size h such as numerical integration, numerical differentiation, numerical methods for solving ordinary and partial differential equations such as Runge-Kutta and finite difference methods respectively. The advantage of implementing the Richardson extrapolation to quadrature rule is to gain a higher accuracy relying on low-order rules and can be efficiently incorporated into Gauss-Type (Mohanty, 2020; Jena and Dash, 2011) and Newton-Cotes-Type quadrature rules (Jena and Dash, 2011).

Furthermore, a simple approach was first proposed by (Das and Pradhan, 1996) combining a pair of quadrature rules of the same degree of precision, say p , producing a mixed quadrature rule of better accuracy, usually $(p + 2)$. They combine the 3-point Gauss-Legendre with Simpson's $1/3$ quadrature rule. It is worth emphasizing that, the formula of the mixed quadrature rule does not involve any extra sampling of the integrand, it only linearly couples the ingredient rules to gain better accuracy. Other formulations of mixed rules are found blending different Gauss-type with Newton-Cotes-Type quadrature rules for approximate evaluation of real definite integral and also for analytic functions (Tripathy et. al., 2015; Patra et. al., 2018; Mohanty, 2010). Such mixed quadrature rules have been implemented to solve singular integral equations in electromagnetic field problems (Jena and Nayak, 2015).

In this paper, three dual hybrid quadrature rules have been constructed for the numerical integration of real definite integrals with singular integrands or non-elementary anti-derivatives. Such quadrature hybridizes between a Newton-Cotes-type formula and a Gauss-type formula enhanced either by Kronrod extension or Richardson extrapolation, both of which have the same degree of precision. This paper is structured as follows: The relevant literature review is presented in Section 1. In Section 2, we introduce some basic definitions. In Section 3, the Kronrod extension of the two-point Gauss-Legendre quadrature rule has been constructed. The open and closed type hybrid rule coupling the Gauss-Kronrod quadrature rule with a derivative-based open and closed type Newton-Cotes rule, respectively, has been formulated in sections 3 and 4. The further closed-type hybrid rule was formulated in Section 5 by combining a numerically enhanced Gauss-Lobatto quadrature rule with Boole's Rule enhanced by Richardson extrapolation. For the sake of verification of the proposed hybrid rules of both types, some numerical results are shown in Section 6, followed by a discussion in Section 7. Finally, a conclusion is drawn in Section 8.

MATERIALS AND METHODS

Basic Definitions

Here we introduce some basic definitions that we need throughout the paper.

Definition 1 [1]: An n -point Gaussian-quadrature rule is defined by the formula,

$$I_n(f) = \int_a^b f(x) dx \cong \sum_{i=1}^n w_i f(x_i) + EI_n(f), \quad (1)$$

where the points x_i are the quadrature points and are known as nodes or abscissas, the factors w_i are the corresponding weights, and $EI_n(f)$ is the error of the rule (1). The quadrature rule (1) is based on polynomial interpolation. The mechanism of the Gauss quadrature is based on the precision concept, that is, the quadrature rule is exact for polynomials of degrees less than or equal to $2n - 1$. That is the formula (1) exactly integrates monomial functions $x^i, i = 0, 1, 2, \dots, n$. Thus we obtain a non-linear system of moment equations that can be solved, yielding the nodes and the corresponding weights.

Definition 2 (Degree of Precision): The degree of precision of the n -point Gaussian-quadrature rule (1) is defined by the degree of the polynomial such that the error $EI_n(P_n) = 0$. Thus the quadrature rule (1) is exact for all polynomials of degree $\leq n$, and the error $EI_n(P_n) \neq 0$ for $i = n + 1, n + 2, \dots$

It is worth emphasizing that for the Newton-Cotes quadrature rules, the equal-distance nodes are known and the weights are unknowns and need to be determined by solving a Vandermonde system, whereas for the Gaussian quadrature rules, the nodes and the weights are both unknowns.

The two-point Gauss-Legendre quadrature rule is given as,

$$I_{GL2}(f) = h \left[f\left(\mu - \frac{h}{\sqrt{3}}\right) + f\left(\mu + \frac{h}{\sqrt{3}}\right) \right], \quad (2)$$

where $h = \frac{b-a}{2}$ and throughout the paper $\mu = \frac{a+b}{2}$ denotes the mid-point of the reintegration interval.

$$I_{Exact}(f) = \int_a^b f(x) dx = I_{GL2}(f) + E_{GL2}(f), \quad (3)$$

Where $E_{GL2}(f)$ is the truncation error of the two-point Gauss-Legendre quadrature. The error can be derived by polynomials interpolation or by Taylor expansion of the functions involved in $I_{GL2}(f)$ about the mid-point μ of the integration interval to yield,

$$E_{GL2}(f) = I_{Exact}(f) - I_{GL2}(f) = \frac{h^5}{135} f^{(4)}(\mu) + \frac{1016h^7}{675 \times 7!} f^{(6)}(\mu) + \dots$$

The degree of precision of the two-point Gauss-Legendre quadrature rule $I_{GL2}(f)$ is three, that is, it should exactly integrate polynomials of degree up to three.

Definition 3 (Stability of Quadrature Rule): If all weights in the formula (1) are non-negative, then the rule is stable and

$$\lambda = \sum_{i=1}^n |w_i| = b - a,$$

where λ is known as the absolute condition number of the quadrature rule.

Definition 4 (Progressive Quadrature Rule): A quadrature rule is called progressive if the nodes for I_{n_1} are also nodes for the successive rule I_{n_2} where $n_2 > n_1$.

The quadrature rule has this outstanding feature that significantly reduces the computational effort for successive quadrature rules by keeping the arithmetic operations that are involved in integrating the integrands to a minimum. Unfortunately, Gauss-Type rules are not progressive; that is Gaussian

rules of different n have no nodes in common except at the midpoint. To overcome this issue, Kronrod (Kronrod;1965) established his progressive extension to the Gauss-Legendre quadrature as shown next.

1 Kronrod Extension of Two-Point Gauss-Legendre Quadrature Rule

The Kronrod extension (Walter, 1988) optimally adds $(n + 1)$ abscissas to the n -point Gaussian rule yielding an $(2n + 1)$ -point Kronrod–Legendre Gauss pair quadrature rule of $(3n + 1)$ or $(3n + 2)$ as degree of precision depending on whether n is even or odd respectively. The $(2n + 1)$ -point Kronrod–Legendre-Gauss pair quadrature $I_{2n+1}(f)$ is progressive as it only requires sampling of the integrand at the new $(n + 1)$ points.

Now we show how to enhance the degree of precision of $I_{GL2}(f)$ seeking its Kronrod extension. Such extension can be achieved by adding three new abscissa to the $I_{GL2}(f)$ in equation (2); that is, we have,

$$I_{KGL2}(f) = \sum_{i=1}^5 c_i f(x_i),$$

where, $x_2 = \mu - \frac{h}{\sqrt{3}}$, and $x_4 = \mu + \frac{h}{\sqrt{3}}$.

To force this quadrature rule to exactly integrate polynomials of degree $3n + 1 = 7$, where $n = 2$, we need to consider the monomial functions $f(x) = x^j, j = 0, 1, 2, \dots, 3n + 1$. Thus we have an algebraic non-linear system with eight unknowns $c_1, c_2, c_3, c_4, c_5, x_1, x_3, x_5$, and eight-moment equations, which can be solved to obtain the Kronrod extension of the Gauss-Legendre quadrature rule $I_{KGL2}(f)$ as,

$$I_{KGL2}(f) = \frac{h}{495} \left\{ 98 \left[f\left(\mu - \sqrt{\frac{6}{7}}h\right) + f\left(\mu + \sqrt{\frac{6}{7}}h\right) \right] + 308f(\mu) + 243 \left[f\left(\mu - \frac{1}{\sqrt{3}}h\right) + f\left(\mu + \frac{1}{\sqrt{3}}h\right) \right] \right\}. \quad (4)$$

This formula can be written as,

$$I_{Exact}(f) = I_{KGL2}(f) + E_{KGL2}(f), \quad (5)$$

where $E_{KGL2}(f)$ is the truncation error of the Kronrod-Gauss quadrature rule and can be computed by Taylor expansions of the functions involved in $I_{KGL2}(f)$ to yield,

$$E_{KGL2}(f) = -\frac{8h^9 f^{(8)}(\mu)}{245 \times 9!} - \frac{5672h^{11} f^{(10)}(\mu)}{7^3 \times 11!} - \dots$$

Thus, the Kronrod extension of the two-point Gauss-Legendre rule considerably enhanced the degree of precision from three to seven, and the local truncation error is of the ninth order. It is worth mentioning that the Gauss-Legendre quadrature rule is of open type because all of its nodes are interior points and usually cluster near the endpoints of the integration interval. Efficient computation of improper integrals with singular integrands can be achieved by this rule, either alone or in con-

junction with other open-type Newton-Cotes quadrature formulas, as demonstrated later. As we have just shown, the Gauss-type quadrature rules can be enhanced by their Kronrod extension, whereas the adaptive quadrature rule can be utilized to enhance the approximate results obtained by the Newton-Cotes-type quadrature rules. Next, we briefly give an overview of the adaptive quadrature rule.

2 Adaptive Algorithm

A mathematical integration technique called adaptive quadrature (Stoer and Bulirsch, 1992; Burden and Faires, 2005) is utilized to approximate the definite integral. This technique dynamically adjusts the subintervals and the number of evaluation points based on the behavior of the integrand to achieve an approximation especially when dealing with rapidly changing functions. The steps involved in this adaptive quadrature algorithm are as follows;

Initial setup: Break up the integration interval into multiple subintervals and approximate the integral for each subinterval.

Error Estimation: Compare the results obtained using the quadrature rule to estimate the error in each subinterval, then identify which subintervals have an impact on the error.

Refinement: Reduce the error by dividing the most significant subintervals into smaller subintervals, then perform the integration process again for the subintervals that have been refined.

Termination: Keep repeating these processes till a certain level of accuracy is reached or until a termination criterion is met.

3 Formulation of the Open-Type Hybrid rule coupling the Gauss-Kronrod rule with a Derivative-Based Open-Type Newton-Cotes rule.

Here, we show how to couple two quadrature rules that both have the same degree of precision, say seven, to yield a hybrid rule of the same degree of precision, nine. The ingredients of the open-type hybrid rule are the Kronrod extension of the two-point Gauss-Legendre rule and a derivative-based open-type Newton-Cotes rule for $n = 3$ which is given by Zafar (Zafar 2014),

$$I_{Exact}(f) = \frac{h}{224} \left\{ \begin{aligned} &1805[f(x_1) + f(x_2)] - 1245[f(x_0) + f(x_3)] \\ &+ h \left[\frac{6605}{9} [f'(x_3) - f'(x_0)] + 1315[f'(x_2) - f'(x_1)] \right] \end{aligned} \right\} + \frac{5951 h^9}{1016064} f^{(8)}(\mu) + \dots,$$

where the quadrature points are,

$$x_i = a + (i + 1)h, \quad i = 0, 1, 2, \dots, n,$$

and the step size is defined as:

$$h = \left(\frac{b - a}{n + 2} \right).$$

This formula can be rewritten as,

$$I_{Exact}(f) = I_{NDO}(f) + E_{NDO}(f), \quad (6)$$

where,

$$I_{NDO}(f) = \frac{h}{224} \left\{ \frac{1805[f(x_1) + f(x_2)] - 1245[f(x_0) + f(x_3)]}{9} + h \left[\frac{6605}{9} [f'(x_3) - f'(x_0)] + 1315[f'(x_2) - f'(x_1)] \right] \right\}, \quad (7)$$

and,

$$E_{NDO}(f) = \frac{5951 h^9}{1016064} f^{(8)}(\mu) + \mathcal{O}(h^{11}).$$

It should be noted that the new derivative-based Newton-Cotes formula I_{NDO} has a degree of precision of seven, the local truncation error is of ninth order, and it only needs four interior quadrature points. Thus, I_{NDO} requires the evaluations of the integrand and its first derivative at a lower number of abscissas compared to the classical Newton-Cotes rules.

Now, multiplying equations (5) and (6), respectively, by $\frac{29755}{2}$ and $\frac{8}{35}$ then adding the resulting equations yields the open-type hybrid quadrature rule as follows:

$$I_{OHR}(f) = \frac{70}{1041441} \left[\frac{29755}{2} I_{KGL2}(f) + \frac{8}{35} I_{NDO}(f) \right], \quad (8)$$

where $I_{KGL2}(f)$ and $I_{NDO}(f)$ are respectively, given by equations (6) and (7). The local truncation error of $E_{OHR}(f)$ is of ninth order, that is,

$$E_{OHR}(f) = \mathcal{O}(h^{11}). \quad (9)$$

We already know that the Gauss-Legendre quadrature rule is of open type because all of its nodes are interior points of the integration interval. Combining this rule with a closed-type Newton-Cotes rule can enable the computation of integrals without a closed-form anti-derivative or a non-elementary anti-derivative, as demonstrated below.

4 Formulation of a Closed-Type Hybrid Rule Coupling the Gauss-Kronrod Rule with a Derivative-Based Closed-Type Newton-Cotes Rule.

Furthermore, we can formulate a closed-type quadrature rule with a degree of precision of seven. Let us recall a derivative-based closed-type Newton-Cotes rule for $n = 3$ (Burg, 2012) given as

$$I_{Exact}(f) = \int_a^b f(x) = \frac{h}{224} \left\{ \frac{93[f(a) + f(b)] + 243[f(x_1) + f(x_2)]}{5} + \frac{h}{5} [57[f'(a) - f'(b)] + 81[f'(x_2) - f'(x_1)]] \right\} + \frac{9 h^9 f^{(8)}(\mu)}{313 \times 600} + \dots, \quad (10)$$

where the quadrature points $x_i = a + ih$, $i = 0, 1, 2, \dots, n$, and the step size is $h = \frac{b-a}{n}$, with degree of precision seven. The formula (10) can be rewritten as,

$$I_{Exact}(f) = I_{NDC}(f) + E_{NDC}(f), \quad (11)$$

where the error is given as:

$$E_{NDC}(f) = \frac{9 h^9 f^{(8)}(\mu)}{313 \times 600} + \mathcal{O}(h^{11}).$$

In a similar fashion to the formulation in Section 3, one can easily obtain the following linear combination of equation (6) with equation (11) yielding a closed-type hybrid quadrature rule as,

$$I_{CHR}(f) = \frac{15337}{167011} \left[\frac{3402}{313} I_{KGL2}(f) + \frac{1}{49} I_{NDC}(f) \right],$$

where $I_{KGL2}(f)$, and $I_{NDC}(f)$ are respectively given by equations (6) and (10). The corresponding truncation error of $I_{CHR}(f)$ is,

$$E_{CHR}(f) = \mathcal{O}(h^{11}). \quad (12)$$

Next, we formulate a closed-type hybrid rule by blending two closed quadrature rules.

5 Formulation of The Closed -Type Hybrid Rule Coupling the Numerically Enhanced Gauss-Lobatto Quadrature Rule with Bool's Rule Enhanced by Richardson Extrapolation.

First, let us start with the Gauss-Lobatto quadrature rule.

5.1 Numerically Enhanced Gauss-Lobatto Quadrature Rule

The standard n-point Gauss-Lobatto quadrature rule is given by the following formula,

$$\int_a^b f(x) dx \approx I_{Lob}(f) = c_1 f(a) + \sum_{i=2}^{n-1} c_i f(x_i) + c_n f(b), \quad (13)$$

where the abscissas x_i are the $(i-1)$ th zero of the $P'_{n-1}(x)$, and $P_n(x)$ is the n^{th} degree Legendre polynomial. This rule is closed because both of the endpoints a, b are also taken as quadrature points, and the degree of precision of this rule is $(2n-3)$.

A numerical enhancement of the Gauss-Lobatto quadrature rule (13) was proposed by (Eslahchi et. al. 2005), they claim that their approach yields better approximate results than those obtained by the corresponding standard Gauss-Lobatto quadrature rule. The core idea of their approach is to consider the end-points of the integral as parameters and that the monomial basis functions x^i is extended from $i = 0, 1, 2, \dots, 2n+1$ (for the standard Gauss-Lobatto) to $i = 0, 1, 2, \dots, 2n+3$. Thus the proposed approach is approximately exact for polynomials of degree up to $2n+3$. That is, they proposed the following system,

$$\int_a^b x^i dx = \frac{b^{i+1} - a^{i+1}}{i+1} = \sum_{k=1}^n w_k x_k^i + \alpha a^i + \beta b^i,$$

for $i = 0, 1, 2, \dots, 2n + 3$, and the notations $a, b, \alpha, \beta, x_1, x_2, \dots, x_n, w_1, w_2, \dots, w_n$ are all unknowns, resulting in a non-linear system that has no analytic solution, but a numerical solution can be found. Thus, all the abscissas, the optimal location of endpoints, and the corresponding weights only have numerical values that are tabulated in (Eslahchi et. al 2005). Thus, one needs to rescale the original integral to fit the new optimal endpoints by the following transformation (Eslahchi et al., 2005),

$$\int_a^b f(x) dx = \int_\delta^\tau \psi(x) dx,$$

where,

$$\psi(x) = \left(\frac{\tau - \delta}{b - a}\right) f\left(\frac{(\tau - \delta)x + b\delta - a\tau}{b - a}\right).$$

A numerically enhanced Gauss-Lobatto quadrature rule for $n = 1$ takes the numerical form within a tolerance 10^{-7} (Eslahchi et. al 2005),

$$\int_a^b f(x) dx \approx I_{N\text{Lob}}(f) = 4.7 \times 10^{-9} + 10^{-3} \left[9.3801 \psi(a) + 9.3802 \psi(b) \right] + 37.5206 \psi(2.5022 \times 10^{-3}), \quad (14)$$

where the optimal locations of the endpoints are:

$$a = -2.789016 \times 10^{-2}, b = 2.839074 \times 10^{-2}.$$

Here, we show how to couple two closed quadrature rules, both having the same degree of precision, to yield a more accurate hybrid rule. The ingredients of the hybrid rule are a numerically improved Gauss-Lobatto quadrature rule, and Bool's rule enhanced by Richardson extrapolation.

5.2 Bool's Rule Enhanced by Richardson Extrapolation.

The closed Newton-Cotes quadrature rule for $n = 4$ is (five abscissas) known as Bool's rule, and is defined by the following formula,

$$\int_a^b f(x) \approx I_{\text{Bool}}(f) = \frac{2h}{45} \left\{ 7[f(a) + f(b)] + 32[f(x_1) + f(x_3)] + 12f(x_2) \right\} - \frac{8h^7}{945} f^{(6)}(\mu). \quad (15)$$

The corresponding error is,

$$E_{\text{Bool}}(f) = -\frac{(2h)^7}{21 \times 6!} f^{(6)}(\mu) + \dots,$$

where the quadrature points $x_i = a + ih$, $i = 0, 1, 2, \dots, n$, and the step size is $h = \frac{b-a}{n}$, with degree of precision five. Here we show how to enhance the Bool's rule by Richardson extrapolation. The mechanism of Richardson extrapolation is to begin with an initial approximation at a certain level of refinement, and then compute a successive approximation using a finer level of refinement. Finally, apply the following Richardson extrapolation formula (Zlatev et. al. 2018) yielding an enhanced accuracy of the approximated integral,

$$\int_a^b f(x) dx \approx I_4^{(k)} = \frac{4^k I_{2n}^{(k-1)} - I_n^{(k-1)}}{4^k - 1}, \quad \text{for } n \geq 2^k, k \geq 1. \quad (16)$$

Starting with $k = 1$ in (16) we have

$$I_4^{(1)} = \frac{4I_8^{(0)} - I_4^{(0)}}{3}, \quad (17)$$

where,

$$I_4^{(0)} = I_{Bool}(f).$$

Now for $I_8^{(0)}$ we have nine points, thus

$$I_8^{(0)} = \frac{h}{45} \left\{ 7[f(a) + f(b)] + 32 \left[f\left(a + \frac{h}{2}\right) + f\left(a + \frac{3h}{2}\right) + f\left(a + \frac{5h}{2}\right) + f\left(a + \frac{7h}{2}\right) \right] \right. \\ \left. + 12[f(a+h) + f(a+3h)] + 14f(a+2h) \right\},$$

By substituting $I_4^{(0)}$ and $I_8^{(0)}$ into equation (17), we obtain

$$I_{RBool}(f) = I_4^{(1)}(f) = \frac{2h}{135} \left\{ \begin{aligned} &7[f(a) + f(b)] - 8[f(a+h) + f(a+3h)] \\ &+ 64 \left[f\left(a + \frac{h}{2}\right) + f\left(a + \frac{3h}{2}\right) + f\left(a + \frac{5h}{2}\right) + f\left(a + \frac{7h}{2}\right) \right] \end{aligned} \right\},$$

where the truncation error of the enhanced quadrature rule $I_4^{(1)}$ can be computed by Taylor expansions of the functions involved in $I_4^{(1)}$ to yield,

$$EI_4^{(1)}(f) = \frac{5(2h)^7}{336 \times 6!} f^{(6)}(\mu) + \frac{277(2h)^9}{11520 \times 8!} f^{(8)}(\mu) + \dots,$$

Comparing the error $EI_4^{(1)}(f)$ with $E_{Bool}(f)$, one could notice that the magnitude of the coefficient of the leading term of $EI_4^{(1)}$ has decreased by an amount of $\frac{5}{16}$ compared to the corresponding term in $E_{Bool}(f)$.

For $k = 2$ in (16), we have

$$I_4^{(2)} = \frac{4I_8^{(1)} - I_4^{(1)}}{15}, \quad (18)$$

where,

$$I_8^{(1)} = \frac{h}{135} \left\{ \begin{aligned} &7[f(a) + f(b)] + 32 \left[f\left(a + \frac{h}{4}\right) + f\left(a + \frac{3h}{4}\right) + f\left(a + \frac{5h}{4}\right) + f\left(a + \frac{7h}{4}\right) + f\left(a + \frac{9h}{4}\right) \right] \\ &\quad + f\left(a + \frac{11h}{4}\right) + f\left(a + \frac{13h}{4}\right) + f\left(a + \frac{15h}{4}\right) \\ &+ 12 \left[f\left(a + \frac{h}{2}\right) + f\left(a + \frac{3h}{2}\right) + f\left(a + \frac{5h}{2}\right) + f\left(a + \frac{7h}{2}\right) \right] \\ &+ 14[f(a+h) + f(a+2h) + f(a+3h)] \end{aligned} \right\}.$$

Substituting $I_4^{(1)}$ and $I_8^{(1)}$ into equation (18) yields,

$$I_4^{(2)} = \frac{2h}{2025} \left\{ \begin{aligned} &77[f(a) + f(b)] + 384 \left[f\left(a + \frac{h}{4}\right) + f\left(a + \frac{3h}{4}\right) + f\left(a + \frac{5h}{4}\right) + f\left(a + \frac{7h}{4}\right) + f\left(a + \frac{9h}{4}\right) \right] \\ &\quad + f\left(a + \frac{11h}{4}\right) + f\left(a + \frac{13h}{4}\right) + f\left(a + \frac{15h}{4}\right) \\ &+ 80 \left[f\left(a + \frac{h}{2}\right) + f\left(a + \frac{3h}{2}\right) + f\left(a + \frac{5h}{2}\right) + f\left(a + \frac{7h}{2}\right) \right] + 176[f(a+h) + f(a+2h) + f(a+3h)] \end{aligned} \right\},$$

the truncation error of the enhanced quadrature rule $I_4^{(2)}$ and can be computed similarly to the error of $I_4^{(1)}$, so

$$EI_4^{(2)}(f) = -\frac{9(2h)^7}{8960 \times 6!} f^{(6)}(\mu) - \frac{421(2h)^9}{245760 \times 8!} f^{(8)}(\mu) - \dots,$$

A similar process can be followed for $k = 3$.

To prevent repetition, in a similar analogy to the derivation in Sections 3 and 4, one could linearly combine the numerically enhanced Gauss-Lobatto quadrature rule with Bool's rule enhanced by Richardson extrapolation, yielding a closed-type quadrature rule $I_{CBoLob}(f)$, and the corresponding truncation error is,

$$E_{CHR}(f) = \mathcal{O}(h^9). \quad (19)$$

RESULTS

Some integral examples are presented in Table (1) to verify the efficiency of the open-type mixed quadrature rule $I_{OHR}(f)$. For example, the following logarithmic integral has non-elementary anti-derivative as:

$$I_1 = \int_1^2 \ln[\ln(x)] dx = -\text{Li}(2) + \gamma + 2 \log(\log 2) \approx -1.20097,$$

where $\text{Li}(x) = \int_0^x \frac{dy}{\ln(y)}$ is the logarithmic integral function, and γ is the Euler–Mascheroni constant; thus such an integral only has a numerical value. Other integral examples of singular-kernel are presented, such as elliptic integral I_2 , exponential integral I_3 , error function I_6 , Dirichlet integral I_7 (Kober, 1940), and incomplete gamma function I_4 . Concerning the Dirichlet integral I_7 , we need the variable transformation $w = e^{-x}$ to transform the indefinite integral I_7 to a definite integral as follows:

$$I_7 = \int_0^\infty \frac{\sin x}{x} dx \xrightarrow{x=\ln\left(\frac{1}{w}\right)} \int_0^1 \frac{\sin\left[\ln\left(\frac{1}{w}\right)\right]}{w \ln\left(\frac{1}{w}\right)} dw.$$

Now, we recall the following transformation:

$$\int_a^b f(w) dw = \int_{-1}^1 f\left[\frac{(b-a)x + b + a}{2}\right] \left(\frac{b-a}{2}\right) dx,$$

Thus, one has

$$\int_0^\infty \frac{\sin x}{x} dx = \int_{-1}^1 \frac{\sin\left[\ln\left(\frac{2}{x+1}\right)\right]}{(x+1) \ln\left(\frac{2}{x+1}\right)} dx.$$

Also, some integral examples of the closed-type mixed quadrature rule are presented in Table (2) to verify the efficiency of the closed-type mixed quadrature rule $I_{CHR}(f)$. For example, the following logarithmic integral has non-elementary anti-derivative:

$$I_1 = \int_1^2 e^{e^x} dx = Ei(e^2) - Ei(e) \approx 255.676,$$

where $Ei(x) = -\int_{-x}^{\infty} \frac{e^{-y}}{y} dy$ is the exponential integral, thus the integral I_1 only has an approximate value. These approximate integral values are used for verification purposes by comparing them with the numerical results obtained by the proposed rules and are referred to as near-exact values. Other integral examples of non-elementary anti-derivatives are also presented, such as the Gaussian integral I_2 (encountered in probability density), the sine integral, and the exponential integral I_4 .

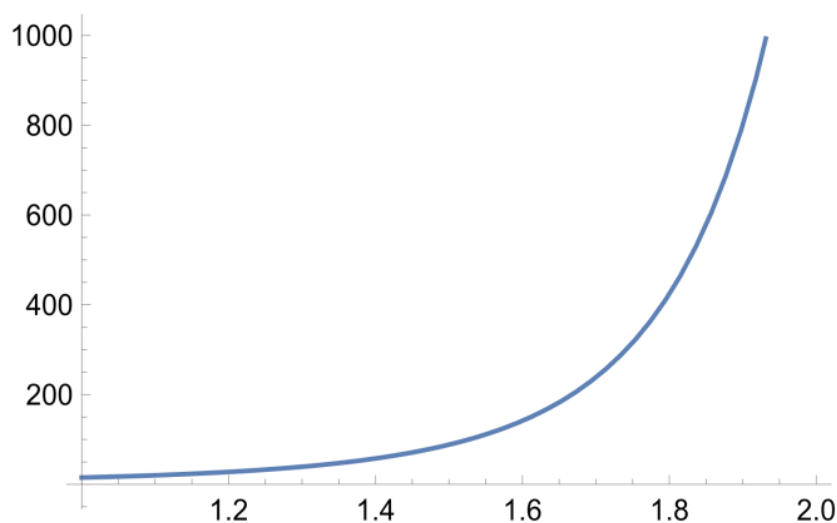


Figure (1): The function $f(x) = e^{e^x}$ along the interval $[0, 2]$

Table: (1). Numerical results computed by the open-type hybrid quadrature rule $I_{OHR}(f)$ compared with its constituent rules $I_{KGL2}(f)$ rules and $I_{NDO}(f)$.

Integral/Transformed Int.	Near-Exact	$I_{KGL2}(f)$	$I_{NDO}(f)$	$I_{OHR}(f)$	Relative Error
$I_1 = \int_1^2 \ln[\ln(x)] dx$	≈ -1.20097	-1.186269827214	-1.150942419465	-1.186203619128	$E_{KGL2} = 1.224350377214 \times 10^{-2}$ $E_{NDO} = 4.165913561106 \times 10^{-2}$ $E_{OHR} = 1.2298632432924 \times 10^{-2}$
$I_1 = \frac{1}{2} \int_{-1}^1 \ln \left[\ln \left(\frac{x+3}{2} \right) \right] dx$	≈ 0.8740191847	0.8747043456216	0.8787134586882	0.8747118592129	$E_{KGL2} = 7.839197005632 \times 10^{-4}$ $E_{NDO} = 5.37090490231107 \times 10^{-3}$ $E_{OHR} = 7.925162982014 \times 10^{-4}$
$I_2 = \int_0^1 \sqrt{1-x^4} dx$					
$I_2 = \frac{1}{8} \int_{-1}^1 \sqrt{16-(x+1)^4} dx$					
$I_3 = \int_1^\infty \frac{e^{-x}}{x} dx$	≈ 0.219384	0.21841054884110	0.23028552760062	0.21843280407190	$E_{KGL2} = 4.43690444836492 \times 10^{-3}$ $E_{NDO} = 4.9691848380501 \times 10^{-2}$ $E_{OHR} = 4.335460234298 \times 10^{-3}$
$I_3 = \int_{-1}^1 \frac{e^{-\left(\frac{2}{1+x}\right)}}{1+x} dx$					
$I_4 = \int_0^\infty e^{-x} x dx$	$\Gamma(2) = 1$	0.9852958834667177	0.9499682436581703	0.9852296749459611	$E_{KGL2} = 1.47041165332823 \times 10^{-2}$ $E_{NDO} = 5.00317563418297 \times 10^{-2}$ $E_{OHR} = 1.477032505403886 \times 10^{-2}$
$I_4 = \frac{1}{2} \int_{-1}^1 \ln \left(\frac{2}{x+1} \right) dx$					
$I_5 = \int_0^\infty \frac{e^{-x}}{1+x^2} dx$	≈ 0.62145	0.621317534623	0.6232082213946	0.6213210780121	$E_{KGL2} = 2.125507968272 \times 10^{-4}$ $E_{NDO} = 2.8298305931829 \times 10^{-3}$ $E_{OHR} = 2.0684898452106 \times 10^{-4}$
$I_5 = 2 \int_{-1}^1 \frac{\left[e^{-\left(\frac{1+x}{2}\right)} + e^{-\left(\frac{2}{1+x}\right)} \right]}{x^2 + 2x + 5} dx$					
$I_6 = \operatorname{Erfc}(1) = \frac{1}{\sqrt{2\pi}} \int_1^\infty e^{-x^2/2} dx$	≈ 0.15865525	0.1587331354611	0.15817808821860	0.1587320952315	$I_{KGL2} = 4.908852857186 \times 10^{-4}$ $I_{NDO} = 3.0075632607556 \times 10^{-3}$ $I_{OHR} = 4.8432874516111 \times 10^{-4}$
$I_6 = \frac{1}{\sqrt{2\pi}} \int_{-1}^1 \frac{e^{-\left[\ln\left(\frac{2e}{x+1}\right)\right]^2/2}}{1+x} dx$					
$I_7 = \int_0^\infty \frac{\sin x}{x} dx$	$= \frac{\pi}{2} \approx 1.5708$	1.6085019683186124	2.076910604996239	1.609379826084149	$E_{KGL2} = 2.3553490365081 \times 10^{-2}$ $E_{NDO} = 2.60795542073356 \times 10^{-1}$ $E_{OHR} = 2.30205838669871 \times 10^{-2}$
$I_7 = \int_{-1}^1 \frac{\sin \left[\ln \left(\frac{2}{x+1} \right) \right]}{(x+1) \ln \left(\frac{2}{x+1} \right)} dx$					

Table: (2). Numerical results computed by the closed-type hybrid quadrature rule $I_{CHR}(f)$ compared with its constituent rules $I_{KGL2}(f)$ rules and $I_{NDC}(f)$.

Integral	Near-Exact	$I_{KGL2}(f)$	$I_{NDC}(f)$	$I_{CHR}(f)$	Relative Error
$I_1 = \int_1^2 e^{e^x} dx$	≈ 255.6758679186	255.820070562722	253.89134362084	255.81645588145	$E_{KGL2} = 5.6400568941 \times 10^{-4}$ $E_{NDC} = 6.9796352399 \times 10^{-3}$ $E_{CHR} = 5.4986794034 \times 10^{-4}$
$I_2 = \int_1^2 e^{-x^2} dx$	$\approx 0.1352572579499946$	0.13525734814014	0.13525655014006	0.1352573466445	$E_{KGL2} = 6.6680450970 \times 10^{-7}$ $E_{NDC} = 5.2330623751 \times 10^{-6}$ $E_{CHR} = 6.55747403635 \times 10^{-7}$
$I_3 = \int_1^2 \frac{\sin x}{x} dx$	$\approx 0.6593299064355118$	0.6593299064397252	0.6593299064006406	0.659329906439652	$E_{KGL2} = 6.3904387767 \times 10^{-12}$ $E_{NDC} = 5.288887503 \times 10^{-11}$ $E_{CHR} = 6.2793036395 \times 10^{-12}$
$I_4 = \int_1^2 \frac{e^{-x}}{x} dx$	≈ 0.170483	0.17048364153294074	0.1704813324558944	0.17048363720543466	$E_{KGL2} = 1.27781034023 \times 10^{-6}$ $E_{NDC} = 1.226648034 \times 10^{-5}$ $E_{CHR} = 1.2524266050 \times 10^{-6}$
$I_5 = \int_0^1 \frac{dx}{1+x^4}$	≈ 0.86697	0.8669767626543958	0.8669225103807843	0.8669766609786879	$E_{KGL2} = 4.3545929803 \times 10^{-6}$ $E_{NDC} = 5.8222066735 \times 10^{-5}$ $E_{CHR} = 4.23731630684 \times 10^{-6}$

Table: (3). Numerical results computed by the closed-type hybrid quadrature rule $I_{CBoLob}(f)$ compared with its constituent rules $I_{RBool}(f)$ rules and I_{NLob} .

Integral	$I_{RBool}(f)$	$I_{NLob}(f)$	I_{CBoLob}	Relative Error
$\int_1^2 e^{-x^2} dx$	0.1352600678077	0.1352461059959	0.135246113746	$E_{RBool} = 2.0774173353466 \times 10^{-5}$ $E_{NLob} = 8.2449949905523 \times 10^{-5}$ $E_{CBoLob} = 8.239264762395 \times 10^{-5}$
$\int_1^2 \frac{\sin x}{x} dx$	0.659329912197	0.6593298963945	0.659329900299	$E_{RBool} = 8.739114546289 \times 10^{-9}$ $E_{NLob} = 8.2449949905523 \times 10^{-5}$ $E_{CBoLob} = 8.2392647623949 \times 10^{-5}$
$\int_1^2 \frac{e^{-x}}{x} dx$	0.170475250379	0.1705180434985	0.1705180554623	$E_{RBool} = 4.7941954266458 \times 10^{-5}$ $E_{NLob} = 2.03068488283273 \times 10^{-4}$ $E_{CBoLob} = 2.0313866405311 \times 10^{-4}$

Table: (4). Numerical results computed by the Closed-type hybrid quadrature rule $I_{CHR}(f)$ compared with its constituent rules and $I_{KGL2}(f)$ rules and $I_{NDC}(f)$ using an adaptive algorithm with termination criterion 10^{-5} .

Integral	Iterations $I_{KGL2}(f)$	Iterations	Iterations $I_{NDC}(f)$	Iterations	Iterations $I_{CHR}(f)$	Iterations
$I_1 = \int_1^2 e^{e^x} dx$	255.675894812	2	255.667210454	12	255.675608551	10
$I_2 = \int_1^2 e^{-x^2} dx$	0.135257258	1	0.135249563462	6	0.135254562	1
$I_3 = \int_1^2 \frac{\sin x}{x} dx$	0.659329906	1	0.659336124	6	0.659330466	1
$I_4 = \int_1^2 \frac{e^{-x}}{x} dx$	0.170480601	1	0.170479739	9	0.170480601391	1

Table: (5). Numerical results computed by the open-type hybrid quadrature rule $I_{OHR}(f)$ compared with its constituent rules $I_{KGL2}(f)$ rules and $I_{NDO}(f)$ using adaptive algorithm.

Integral	$I_{KGL2}(f)$	Iterations	$I_{NDO}(f)$	Iterations	$I_{CHR}(f)$	Iterations
$I_1 = \int_1^2 \ln[\ln(x)] dx$	-1.2009667766545051	10	-1.200967848901904	12	-1.20096674432545	10
$I_2 = \int_0^1 \sqrt{1-x^4} dx$	0.8740193510435356	7	0.8740193218057818	9	0.8740193527868432	7
$I_5 = \int_0^\infty \frac{e^{-x}}{1+x^2} dx$	0.621449500800718	1	0.6214593348845058	12	0.6214519128864372	5
$I_7 = \int_0^\infty \frac{\sin x}{x} dx$	1.5888888194648858	13	1.5689338860146185	10	1.5886295131152703	13

DISCUSSION

For numerical computations, we build up some numerical routines by Mathematica 3.1. software. Table (1) shows the approximate values of some improper integrals, either with singular integrands or with infinite intervals of integration. With a small number of abscissas, the observed accuracy is quite good and very satisfactory. It should be noted that the relative errors related to the approxi-

mate results shown in Tables (2) and (3) are much smaller than those in Table (1). This variance between both categories can be traced back to the fact that the integrands in Table (2) are quite well-behaved functions, unlike the integrands in Table (1) which can be considered bad-behaved functions. For instance, the Dirichlet integral I_7 in Table (1) has a singularity at both endpoints of the integration interval. Also, the integrand of I_1 in Table (2) experiences very sharp variations, especially in the sub-region (1.5,2) as shown in Figure (1). Thus, to achieve higher accuracy for $I_{OHR}(f)$, the rule $I_{NDO}(f)$ needs to be enhanced by an adaptive algorithm. Thus, one urgently needs a local-adaptive algorithm for $I_{NDO}(f)$ and $I_{NDC}(f)$ to conveniently capture the integrand behavior rather than only relying on four nodes. However, such integrand behavior will be inherited in the adaptive algorithm; the adaptive quadrature algorithm for integrals in Table (1) may suffer from slow convergence and thus need quite a few iterations, as shown in Table (4). Tables (4) and (5) show that the approximate results agree with the near-exact ones up to four digits as we set up the termination criterion of the adaptive algorithm to 10^{-5} .

CONCLUSION

Open and closed hybrid quadrature rules $I_{OHR}(f)$, $I_{CHR}(f)$, and $I_{CBoLob}(f)$ have been proposed in this paper. Their ingredients are some enhanced quadrature rules, such as the Kronrod-Legendre pair, Bool's rule enhanced by Richardson extrapolation, the numerically enhanced Gauss-Lobatto quadrature rule, and derivative-based Newton-Cotes formulae. The proposed hybrid quadrature rules are found to

perform better than their ingredient quadrature rules through error analysis, as evidenced in equations (9), (12), and (19). Strictly speaking, the degree of precision of the proposed hybrid quadrature rules is $(p + 2)$, where p is the degree of precision of its ingredient rules. A variety of integral examples have been considered for verification purposes that correspond to numerous applications in science and engineering. Considering that we implement low-order quadrature rules of either the Gauss or Newton-Cotes type, the observed accuracy is satisfied. The performance of such hybrid rules can be enhanced by the adaptive quadrature rule as shown in Tables (4) and (5) with a tolerance of 10^{-5} . Overall, all the results obtained are very satisfactory.

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

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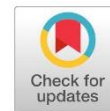
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Research Article

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Synthesis and Antimicrobial Activity of Zinc(II) Complexes of Schiff Bases Derived from 2-Aminobenzoic Acid

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Abstract

Research in Schiff base complexes has been among the most intriguing areas in coordination chemistry. Mononuclear zinc Schiff base complexes of the type $[Zn(L1)(H_2O)_2]$ and $[Zn(HL2)_2]$ and dinuclear complexes of the type $[Zn_2(L1)Q(OAc)(H_2O)]$ and $[Zn_2(L2)Q(OAc)(H_2O)]$ (where $H_2L1 = 2,2'-(2-hydroxybenzylidene)amino$ benzoic acid, $H_2L2 = 2,2'-(4-hydroxy-3-methoxybenzylidene)amino$ benzoic acid and $HQ = 8-hydroxyquinoline$) are described. The complexes were investigated by using various spectroscopic methods including elemental analysis, mass spectra, 1H -NMR spectra, Fourier transform infrared (FT-IR) and UV-visible spectra. Using the diffusion method, the Schiff bases and Schiff base zinc complexes were screened in vitro against four bacteria (*S. aureus*, *K. pneumoniae*, and *Acinetobacter* spp. and *E. coli*).

Keywords: 2-aminobenzoic acid; Zinc (II) complexes; 8-hydroxyquinoline Ligand, Spectrophotometry; Antibacterial

INTRODUCTION

Schiff base metal complexes have been playing an important role in coordination chemistry development due to the simple and direct synthesis of quite different ligands, reactivity, versatility and richness of the chemistry, stability of the complexes and their fascinating potential applications (Abu-Dief & Mohamed, 2015; Gupta & Sutar, 2008). Schiff base complexes play vital roles in modern coordination chemistry in addition to the improvement of bioinorganic chemistry (Deghadi *et al.*, 2022), catalysis (Dalia *et al.*, 2018; Cozzi, 2004) and magnetism (Rani *et al.*, 2018). Schiff base type ligands in coordination chemistry are flexible ligands that can confer better coordination tendency to a metal center in different coordination modes. They commonly coordinate to metal centers through azomethine nitrogen with other donor atoms from carbonyl moiety yielding mono or polynuclear complexes. However, the chelation capacity of the Schiff base ligand can be increased by introducing additional donor atoms ((Rani *et al.*, 2018; Abdel-Rahman *et al.*, 2019)). Among Schiff bases ligands, N, O type ligands have attracted considerable attention because of the stability that they give to their complexes by chelation (El-t Ashoor & Shawish, 2015; Lazzarini *et al.*, 2016).

Schiff bases that are derived from 2-aminobenzoic acid have gained significant attention. These ligands coordinate with the metal ions as anionic NO and NOX (where X = O, N, or S) chelating



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ligands. In the NO mode, the coordination occurs through the imine nitrogen and oxygen atoms of the carboxylic group to form mononuclear complexes with the ligand binding to the metal center forming one six-membered ring (Abdel-Rahman *et al.*, 2019; Jirjees *et al.*, 2021). Whereas, the NOX donor ligands coordinate to the metal center through the imine nitrogen, oxygen of the carboxylic group and the X atom attached to the aldehyde/ketone skeletal forming mononuclear or dinuclear complexes (Wu *et al.*, 2020).

Interest has centered on zinc(II) complexes with N, O bidentate donor ligands due to the ability of zinc to bind to hard donors. Generally, Zinc in biological systems is mainly coordinated with nitrogen and oxygen of amino acid residues (Pellei *et al.*, 2021). Moreover, certain zinc complexes with N, O type ligands exhibit considerable biological activities. Dasgupta *et al.*, It has been reported that Zn (II) complexes with acyl hydrazone Schiff base ligands exhibit anti-cancer activity towards (human colorectal carcinoma) HCT116, (human hepatocellular carcinoma) HepG2, and (human non-small lung carcinoma) cell lines A549. (Dasgupta *et al.*, 2020).

In this study, the aim was to present the synthesis and structural characterization of zinc (II) complexes with Schiff base derivatives of 2-aminobenzoic acid. The Schiff bases (H_2L^1 and H_2L^2) react with zinc(II) acetate dihydrate to afford a mononuclear zinc complex. However, the reaction of these Schiff bases with $Zn(OAc)_2 \cdot 2H_2O$ in the presence of 8-hydroxyquinoline afforded binuclear complexes and the antibacterial activity of the complexes has been evaluated.

MATERIALS AND METHODS

Reagents and solvents

All reagents and solvents were obtained from commercial sources and used without further purification. 2-aminobenzoic acid, salicylaldehyde and 3-methoxy 4-hydroxybenzaldehyde have been acquired from Alfa Aesar, 8-hydroxyquinoline was supplied from Riedel-De Haen, zinc (II) acetate dihydrate was supplied from Merck. The ligands H_2L^1 and H_2L^2 have been synthesized according to the previously published procedure (El-Ajaily *et al.*, 2016).

Physical measurements

The equipment used for elemental analysis was the Perkin Elmer Model 2400. Perkin Elmer FT-IR Spectrometer (Frontier) where used for infrared spectra. The UV-Vis spectra for the metal complexes in the DMSO solution were recorded in the 200–800 nm range on an Agilent Technologies Cary 60 UV-Vis spectrophotometer. Mass spectra (EI) were recorded using a micromass autospec spectrometer. JEOL JNM-ECA Series FT NMR was used to document 1H -NMR spectra.

Synthesis of the complexes

Synthesis of the complexes $[ZnL^1(H_2O)_2]$ (C1) and $[Zn(HL^2)_2]$ (C2)

A solution of $Zn(CH_3COO)_2 \cdot H_2O$ (0.5 mmol, 0.1097 g) in 20 mL of methanol was added to a solution of the ligand H_2L^1 (1 mmol, 0.241 g) or H_2L^2 (1 mmol, 0.271 g) dissolved in 20 mL of methanol. The mixture was heated to reflux for 4 hours. The resulting precipitates were filtered then washed with water, methanol and then dried at room temperature.

Synthesis of the complexes $[ZnL^1Q(OAc)(H_2O)]$ (C3) and $[Zn(L^2)Q(OAc)(H_2O)]$ (C4)

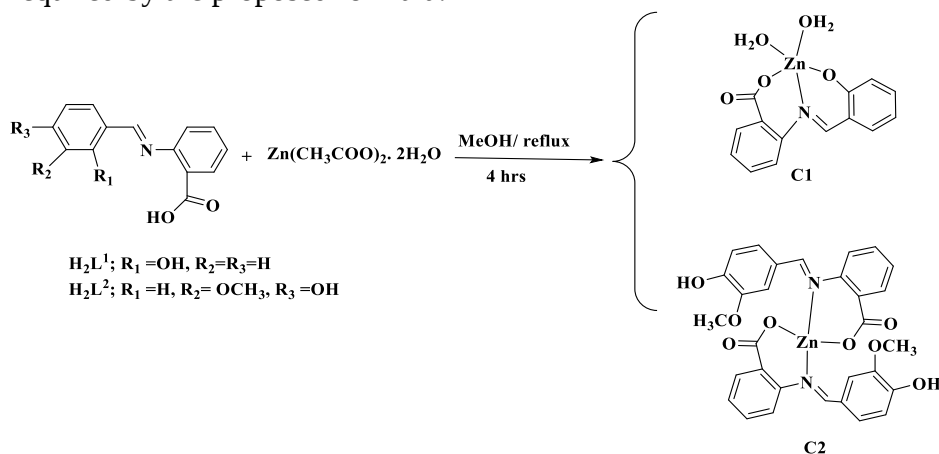
In a 5 mL methanol solution, 1 mmol (1.45g) of 8-hydroxyquinoline was mixed with either 1 mmol (0.241g) of Schiff base ligand H_2L^1 or 1 mmol (0.271g) of H_2L^2 Schiff base ligand, dissolved in 20 mL methanol. Next, a solution of $Zn(CH_3COO)_2 \cdot H_2O$ (1mmol, 0.219g) in 20 mL methanol was added. The mixture was heated and stirred for 5 hours. The resulting suspension was filtered washed with methanol then dried in air.

Antibacterial study

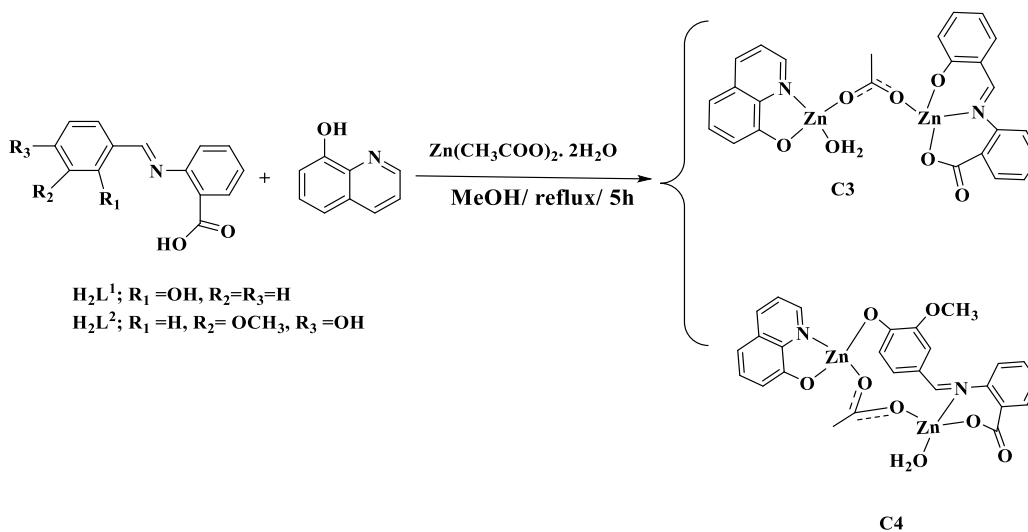
The Schiff bases H_2L^1 and H_2L^2 , along with zinc (II) complexes, were tested against bacterial strains: *Acinetobacter* spp., *Staphylococcus aureus*, *Streptococcus*, *Klebsiella pneumonia*, and *Escherichia coli* by using the agar-well diffusion method (Bauer, 1996). The antibacterial efficiency was tested using the DMSO as solvent. The tested compounds were added to agar plates, which were then incubated at 37 °C for 24 hours. The inhibition zones were measured in millimeters, and the experiment was repeated twice to ensure accuracy.

RESULTS

The mononuclear zinc (II) complexes C1 and C2 are prepared from a typical synthetic procedure, in which $Zn(OAc)_2 \cdot 2H_2O$ is reacted with Schiff bases H_2L^1 and H_2L^2 in methanol aqueous (Scheme 1), while the dinuclear mixed ligand complexes C3 and C4 are prepared with the Schiff bases in the presence of 8-hydroxyquinoline as a co-ligand (Scheme 2). The prepared complexes are air stable, soluble in DMSO, DMF and almost insoluble in water and other common organic solvents as well. The physical properties and analytical data of the prepared complexes are summarized in Table 1. The elemental analysis results of the prepared complexes are in good agreement with the results required by the proposed formula.



Scheme (1). Schematic routes of the synthesis of complexes C1 and C2



Scheme (2). Schematic routes of the synthesis of complexes C3 and C4

Table (1). Analytical data of the ligand–metal complexes

Compound	Molecular Formula	Colour	Melting Point °C	Yield (%)	Anal.Calc. (Found)%		
					N	H	C
[ZnL ¹ (H ₂ O) ₂](C1)	C ₁₄ H ₁₄ NO ₅ Zn	Pale yellow	280	68	4.11 (4.01)	4.40 (4.02)	49.36 (49.10)
[Zn(HL ²) ₂](C2)	C ₃₀ H ₄₀ N ₂ O ₈ Zn	Pale yellow	285	72	4.62 (4.60)	3.99 (4.06)	59.47 (59.44)
[ZnL ¹ Q(OAc)(H ₂ O)](C3)	C ₂₅ H ₂₀ N ₂ O ₇ Zn ₂	Yellow	Up to 300	44	4.74 (4.78)	3.41 (3.80)	50.79 (51.02)
[ZnL ² Q(OAc)(H ₂ O)](C4)	C ₂₆ H ₂₂ N ₂ O ₈ Zn ₂	Pale yellow	Up to 300	48	4.51 (4.35)	3.57 (3.43)	50.27 (50.12)

IR spectra of the prepared complexes were compared with those of their free Schiff bases H₂L¹ and H₂L² (Table 2). The bands at 1688 and 1690 cm⁻¹ in the spectra of free H₂L¹ and H₂L² ligands can be attributed to the C=O stretching of the carboxylic group. However, these bands disappeared in the spectra of the zinc complexes and new bands at around 1540 cm⁻¹ and 1370-1407 cm⁻¹ which attributed to $\nu_{as}(\text{COO}^-)$ and $\nu_s(\text{COO}^-)$, respectively (Refat *et al.*, 2013; Dubey & Mishra, 2011). Also, the IR spectra of the free ligands presented distinguishing bands at 1615 and 1593 cm⁻¹ for the CH=N, which were moved downfield to 1593 and 1589 cm⁻¹ upon complexation of ligands H₂L¹ and H₂L², respectively, hence elucidating the coordination of N atom of the CH=N group to the central zinc (II) ion (Aldawood, 2013). Coordination of the phenolic oxygen to zinc (II) ion in C1, C3, and C4 complexes is confirmed by the shift of the strong band at about 1244 cm⁻¹ in the H₂L¹ and at 1279 cm⁻¹ in H₂L², which is ascribed to C-O stretching vibrations, to lower frequency at 1232 cm⁻¹ (Uba, 2023).

Table (2). IR spectra of the ligands and their zinc complexes

compound	Stretching frequency (cm ⁻¹)								
	$\nu_{\text{C=O}}$	$\nu_{\text{C=N}}$	$\nu_{as}\text{COO}^-$	$\nu_{s}\text{COO}^-$	$\nu_{\text{C-O}}$	$\nu_{\text{C=N}}$ Quinoline	$\nu_{\text{C-O}}$ Quinoline	$\nu_{as}\text{COO}^-$ acetate	$\nu_{s}\text{COO}^-$ acetate
H ₂ L ¹	1688	1615	-	-	1244	-	-	-	-
H ₂ L ²	1690	1589	-	-	1279	-	-	-	-
C1	-	1593	1542	1406	1232	-	-	-	-
C2	-	1591	1540	1407	1272	-	-	-	-
C3	-	1593	1541	1372	1231	1467	1109	1499	1390
C4	-	1593	1543	1387	1235	1467	1110	1499	1387

This band did not shift in the IR spectrum of complex C2, which appeared at 1275 cm⁻¹. This confirms that the phenolic OH group is not coordinating with Zn. (II) (Fugu *et al.*, 2013). Moreover, the IR spectra of the mixed complexes C3 and C4 displayed new bands at 1109 and 1467 cm⁻¹ assignable to $\nu(\text{C-O})$ and $\nu(\text{C=N})$, respectively in the co-ligand 8-hydroxyquinoline. (Shivankar *et al.*, 2003; Bufarwa & Abdel-Latif, 2022). Another new band appeared only in the IR spectra of C3 and C4 at 1499 and 1390 cm⁻¹ assigned for $\nu_{as}(\text{COO}^-)$ and $\nu_s(\text{COO}^-)$ in the acetate group, indicating the involvement of acetate as a bridging ligand (Nakamoto, 2009). When used in conjunction with other spectroscopic information, ¹H NMR is a valuable tool for identifying coordination sites in zinc (II) complexes. The chemical shifts of the Schiff base ligands and their zinc complexes

[ZnL¹(H₂O)₂] (C₁), [Zn (HL²)₂] (C₂), [ZnL¹Q(OAc)(H₂O)] (C₃) and [Zn(L²)Q(OAc)(H₂O)] (C₄) are presented in Table 3. Figure 1 shows the ¹H NMR spectra for the ligands and their prepared zinc complexes. The singlet band appeared at 10.25 and 9.77 ppm for the free Schiff bases H₂L¹ and H₂L² respectively, and is assigned to the phenolic proton.

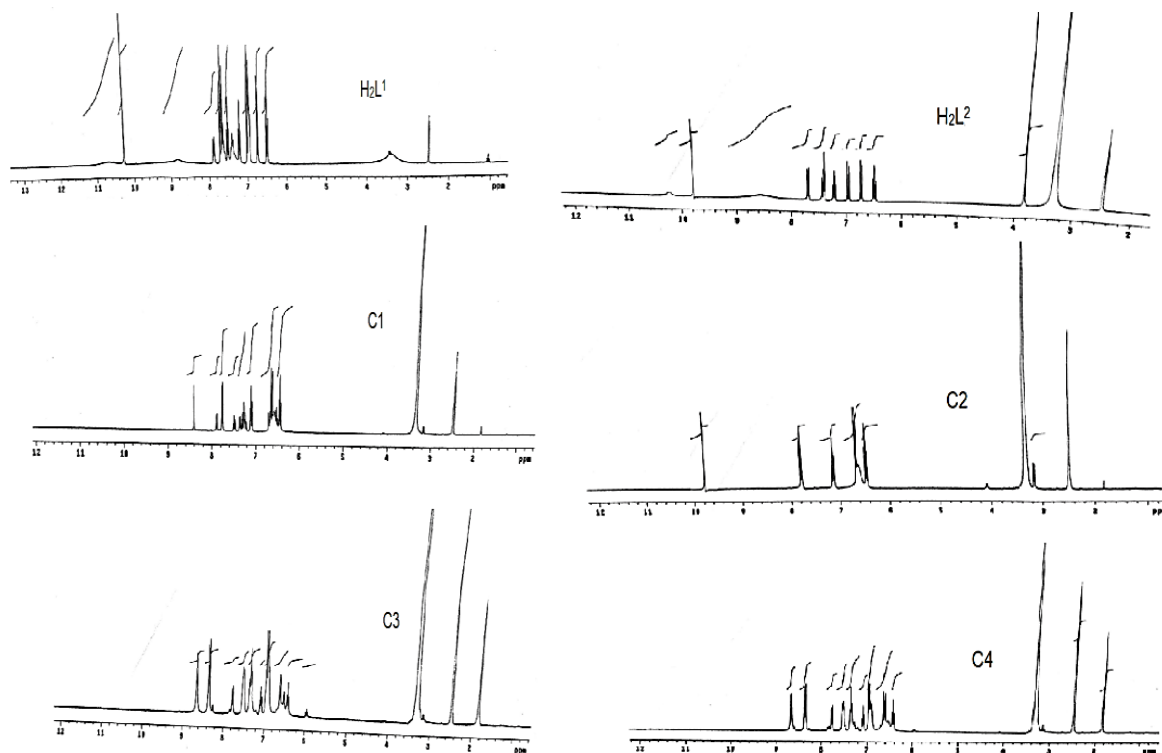


Figure (1). ¹H NMR spectra for the ligands and their prepared zinc complexes

Table (3). ¹H NMR spectral data (δ, ppm) of H₂L¹, H₂L², and their Zn (II) complexes

compound	Chemical shifts, δ (ppm)					
	COOH	OH	C=N	Aromatic	CH ₃ (acetate)	OCH ₃
H ₂ L ¹	10.90	10.25	8.86	7.71- 6.49	-	-
H ₂ L ²	10.30	9.77	8.84	6.49-7.69	-	3.84
C1	-	-	8.47	7.90- 6.42	-	-
C2	-	9.85	7.89	6.44 -7.77	-	3.18
C3	-	-	8.64	6.43-7.19	1.85	-
C4	-	-	8.66	6.41-7.78	1.85	-

This signal is absent from the spectra of complexes C₁, C₃, and C₄, showing that coordination of the ligands H₂L₁ and H₂L₂ to Zn (II) was through the oxygen atom of these ligands with deprotonation (Nishal *et al.*, 2014). Also, the singlet at 10.90 and 10.30 ppm in the free ligands H₂L¹ and H₂L² respectively, which is attributed to the proton of the carboxylic group, disappeared in the ¹H NMR spectra of all complexes. The coordination of the carboxylic oxygen with the zinc center is likely confirmed. In all complexes, the azomethine proton signal in the ¹H NMR spectra is shifted upfield compared to the free ligands, indicating coordination through the azomethine nitrogen. Ad-

ditionally, the singlet at 1.85 ppm corresponds to the CH_3 of the acetate moiety in the C3 and C4 complexes, integrating as three hydrogens (Abu-Dief *et al.*, 2019).

Electronic spectra of the zinc(II) complexes and the free Schiff bases were recorded in DMSO (1×10^{-5} M) at room temperature. The study results are depicted in Figure 2 and Table 4. The Schiff base H_2L^1 exhibits two absorption bands at 261 and 315 nm, respectively attributed to ($\pi \rightarrow \pi^*$) and ($n \rightarrow \pi^*$) transitions of the azomethine and carboxylic chromophore. Similarly, the ligand H_2L^2 exhibits two bands that appeared at 280 and 313 nm which are attributed to the ($\pi \rightarrow \pi^*$) and ($n \rightarrow \pi^*$), respectively. On complexation, this band was shifted to a higher wavelength region, proposing the coordination of azomethine nitrogen and carboxylic oxygen with Zn (II) ion (Belal *et al.*, 2015). Furthermore, complexes C3 and C4 exhibit a broadband at 398 nm, which is assigned to metal-ligand charge transfer (MLCT) transitions. This is expected for zinc complexes (Abdel-Rahman *et al.*, 2017). The mass spectra of the complexes showed different patterns of fragmentation, as expected. The results were consistent with the molecular formulas of the compounds. Figure 3 displays the mass spectra of the C1, C2, C3, and C4 complexes. These spectra showed molecular ion peaks at $m/z = 341, 607, 593, \text{ and } 622$, respectively. These peaks matched the calculated weights of 340.64, 592.21, 605.91, and 621.23.

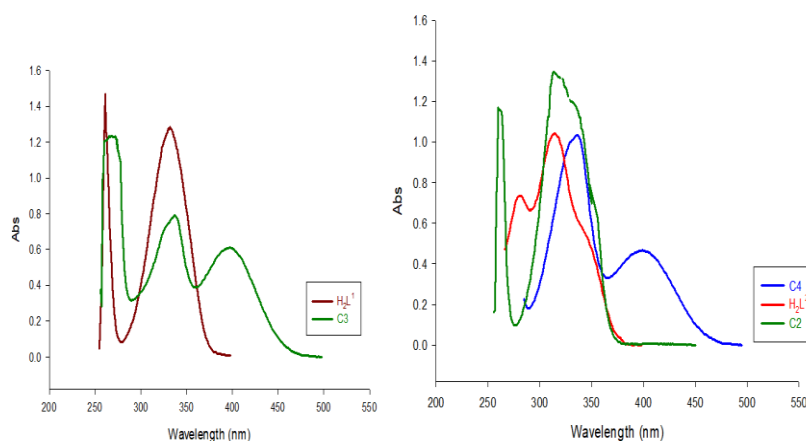


Figure (2). Electronic spectra of the ligands and their zinc (II) complexes

Table (4). Electronic spectra data of the ligands and their zinc (II) complexes

Compound	Absorbance (nm)	Assignment
H_2L^1	259	$\pi \rightarrow \pi^*$
	331	$n \rightarrow \pi^*$
H_2L^2	260, 281	$\pi \rightarrow \pi^*$
	315	$n \rightarrow \pi^*$
C1	266	$\pi \rightarrow \pi^*$
	338	$n \rightarrow \pi^*$
C2	396	$M \rightarrow L$
	272	$\pi \rightarrow \pi^*$
C3	336	$n \rightarrow \pi^*$
	268	$\pi \rightarrow \pi^*$
C4	336	$n \rightarrow \pi^*$
	405	$M \rightarrow L$

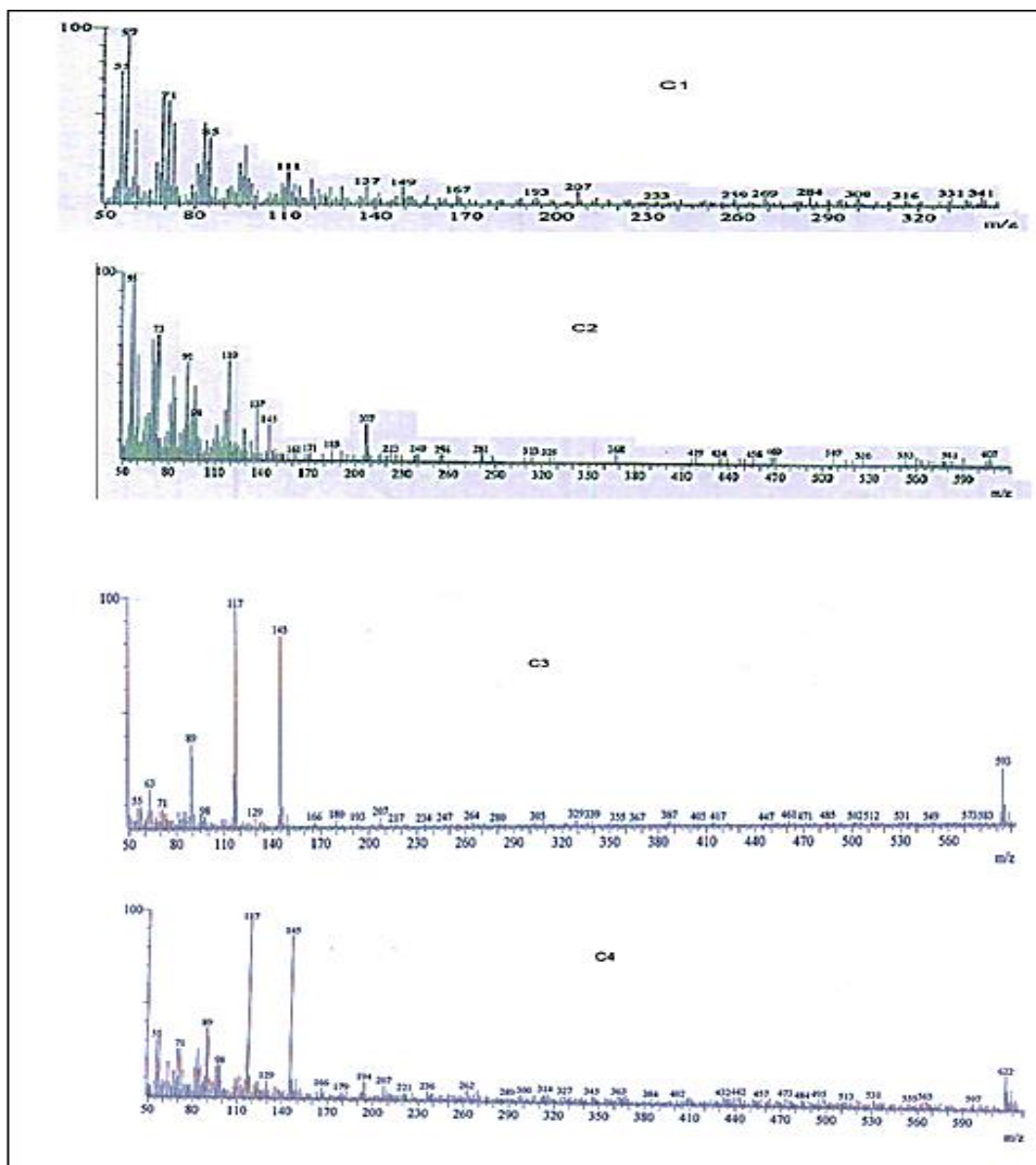


Figure (3). Mass spectra of zinc complexes

The antibacterial potential of the ligands and their zinc (II) complexes is investigated. For antibacterial testing, Gram-negative strains (*Escherichia coli*, *Streptococcus Klebsiella pneumonia*, and *Staphylococcus aureus*) and Gram-positive strains (*Acinetobacter Spp.*) were used. Table 5 summarizes the results of the antibacterial activity. The ligands had low activity against each bacterial species, however, the zinc complexes performed better than the original ligands. All prepared zinc complexes showed notable antibacterial activity against the *Streptococcusaureus* bacterial strain with an inhibition zone range of 14-20. However, the zinc complex $[ZnL^1(H_2O)_2]$ (C1) With an inhibition zone diameter of 20mm, showed demonstrated activity against the *Staphylococcus aureus* strain. This result can be comparable with results reported in the literature (Joseyphus & Nair, 2008; Zabin *et al.*, 2018).

Table (5). shows the antibacterial activity of ligands and their zinc complexes.

Compound	Bacterial Zone of Inhibition (mm)			
	Gram Positive		Gram Negative	
	<i>Staphylococcus aureus</i>	<i>Escherichia coli</i>	<i>Acinetobacter Spp.</i>	<i>Klebsiella pneumonia</i>
DMSO(control)	6	6	6	6
H ₂ L ¹	6	11	7	7
H ₂ L ²	6	11	10	7
C1	20	17	19	15
C2	14	6	11	10
C3	16	14	14	10
C4	19	14	19	14

CONCLUSION

Schiff bases derived from 2-aminobenzoic acid were synthesized and characterized as zinc (II) complexes. Schiff base ligands coordinate with the Zn (II) ion in various ways, including as a dibasic tridentate ONO chelating ligand and as a negative ON bidentate ligand. According to the antibacterial study, Zinc (II) complexes have better antibacterial properties than free Schiff base ligands.

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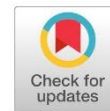
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Research Article

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Size structure and dynamics of the threatened *Laurus nobilis* L population in Shahat, AL-Jabal AL-Akhdar, Libya

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Abstract

The fragrant evergreen leaves of the bay tree, also known as laurel (*Laurus nobilis* L., Lauraceae), are a large shrub that is extensively used in Mediterranean cooking. The present work aimed to study the size structure of *Laurus nobilis* populations concerning their soil conditions. Twenty-one terraces (25m × 25m) were selected at Shahat of Al-Jabal AL-Akhder at three different levels. The height-to-diameter ratio was more than unity for *Laurus nobilis*. This means that the diameter of these species tends to expand vertically rather than horizontally. Five forms of size distribution along the different elevations were recognized. In the present study, it was found that *Laurus nobilis* exhibited more or less J-shaped distribution along elevation levels (downstream and mid-stream). *Laurus nobilis* exhibited more or less symmetrical distribution (bell-shaped) along the elevation level (upstream). The negatively skewed distribution of *Laurus nobilis* indicated the dominance of mature individuals over the juvenile ones. The field observations were consistent with the results of the investigation of soil properties.

Keywords: Population dynamic; Size distribution; *Laurus nobilis* L; Shahat, AL-Jabal AL-Akhdar, Libya .

INTRODUCTION

The Greeks established the ancient city of Shahat, Cyrene (Qurina), in the northeastern Libyan district of Al-Jabal AL-Akhdar. Overall, recent vegetation studies revealed a high degree of plant diversity. Furthermore, the vast majority of Al-Jabal AL-Akhdar's wild plants are used in biotechnology and medicine. There are medicinal plants all over the nation, although they are concentrated in the areas of Al-Jabal AL-Akhdar (UNEP, 2002). However, a shift in the vegetation within this delicate ecosystem may result from various factors, including desertification, increased rates of dry land degradation, overgrazing, urbanization, and the destruction of natural vegetation (MEA, 2005; El-Barasi *et al.*, 2013). Along with extensive human activity, large areas have been reclaimed. Without a doubt, these activities have had a negative impact on species diversity as well as size structure. The ages, sizes, and morphologies of the individuals that make up a plant population can be used to characterize its structure (Harper & White, 1974). The characterize population structure, plant size, and reproductive traits in *Laurus nobilis* commonly known as bay leaves. Its leaves and extracts are used to treat eructation, flatulence, and gastrointestinal issues, as well as to suppress bacterial and fungal infections and high blood sugar. Moreover, it has antioxidant, anti-inflammatory, anticonvulsive, and antiepileptic qualities (Gómez-Coronado & Barbas, 2003;



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Ouchikh *et al.*, 2011; Ramos *et al.*, 2012). The most prevalent phenolic compounds in bay leaves have been reported to be flavonoids, including derivatives of myrcetin, luteolin, apigenin, kaempferol, and quercetin (Lu *et al.*, 2011). The current study set out to examine the dynamics and population structure of *Laurus nobilis* in various habitats in Shahat, North-Eastern Libya.

MATERIALS AND METHODS

Location of study area:

The study area is located in the Mediterranean Sea Cost of Libya between latitude 32°35'52.84" N and longitude 21°28'22" E (Al-Jabal Al-Akhder South project, 2005) Cyrene is located about 10Km east of the city of Al-Bayda, in the northeast of Libya. It is found on the second terrace of Al- Jabal Al- Akhdar, at an elevation of around 600 meters, its height is between (555: 578) meters it lies between Latitude 32°49'23.952 'N And longitude 021°51'11.1888 'E on the North East region, Al Jabal Al-Akhdar (Newport & Haddor, 1963). The study area is shown in Figure 1.

Climate of the area:

The distinctive features of the climate of the study area are a concentration of rainfall during the cool winter season and summer drought climate data for the study area. December and January have the highest mean monthly rainfall totals, at 63 and 62 mm, respectively. The annual rainfall average is roughly 566 mm, albeit highly variable in terms of location. Just before spring, humidity rises, with a peak of 33% in March. In June, the mean maximum monthly temperature reaches 38°C; in January and December, it drops to 21°C and 22°C, respectively. January and December have the lowest mean minimum monthly temperatures, with 5°C and 6°C, respectively (Shahat Meteorological Station). Figure 2 (El-Tantawi, 2005).

Collections and population frequency:

Twenty one quadrates (each of 25x25m) were selected to represent the main habitats of *Laurus nobilis* populations along Shahat. The population structure of these species was evaluated in terms of size distribution. The size index of each individual was calculated as the mean of its height and diameter $[(H+D)/2]$. The size estimates were then used to classify the population into 7 size classes. The size classes (m/ ind.) are (1=0<1, 2=1.1-2, 3=2.1-3, 4=3.1-4, 5=4.1-5, 6=5.1-6 and 7=6.1-7) (Shaltout *et al.*, 2015).

Soil analysis:

In each location, one composite soil sample was collected from soil profiles (0 – 25cm), air dried then physical and chemical parameters of such soil samples were analyzed (Gupta, 2000; Brown, 1998; Allen *et al.*, 1974; Blanchar *et al.*, 1965).

RESULTS

Size distribution analysis of *Laurus nobilis* population using tree height and diameter, the size was estimated by measuring the height and mean diameter were shown in Table 1. Generally, the height to diameter ratio was more than unity for *Laurus nobilis*. The relationships between the individual heights and diameters of the *Laurus nobilis* population are simple linear with r^2 values of 0.616 Figure 3. The population downstream had highest height-to-diameter ratio (5.32), except the population upstream had the lowest (3.22).

In the present study, it was found that *Laurus nobilis* exhibited more or less J-shaped distribution along elevation levels I (downstream and midstream). *Laurus nobilis* exhibited more or less symmetrical distribution (bell-shaped) along the elevation level (upstream). The distribution of *Laurus nobilis* was negatively skewed, indicating that mature individuals outnumbered juvenile ones. Due

to the population's high proportion of larger individuals relative to smaller ones, this distribution is indicative of a declining population. The distribution pattern suggests that there is no recruitment to support the smallest size categories. Furthermore, the study area's high mortality rate is caused by human disturbance, as evidenced by the diminishing numbers of both small and large trees Figure 4.

Soil chemical and physical analysis in different elevation levels indicated that at Shahat, soils elevation downstream were characterized by the highest values of E.C (0.344 ds/m) as well as bicarbonate, sulfate, and sodium (0.75, 5.22 and 6.6 m.eq./L. respectively) Table 2. Soils at midstream were values of clay (58.24), but the lowest value was E.C, silt and chloride (0.144 m.eq./L., 37.51 and 0.71 m.eq./L. respectively). Clay and E.C content in soil showed significant variations between the three levels.



Figure (1): Location map indicating the study

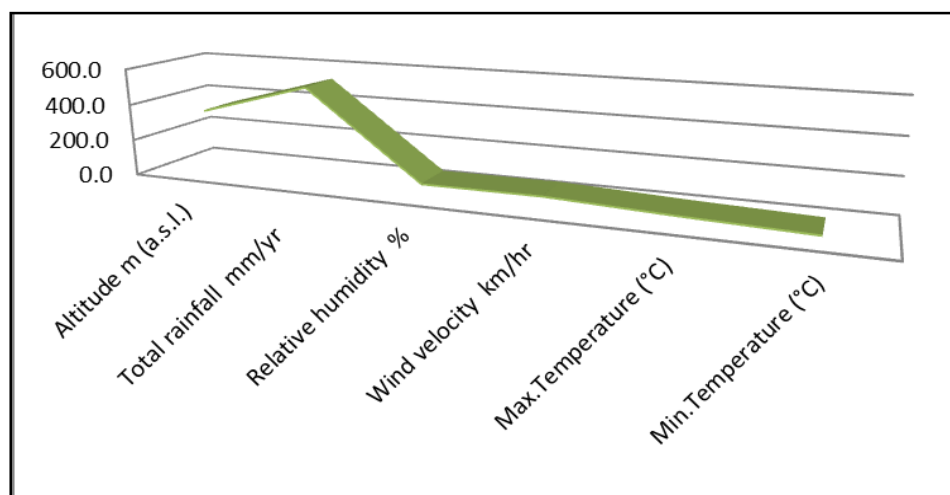


Figure (2): Meteorological data of Shahat station.

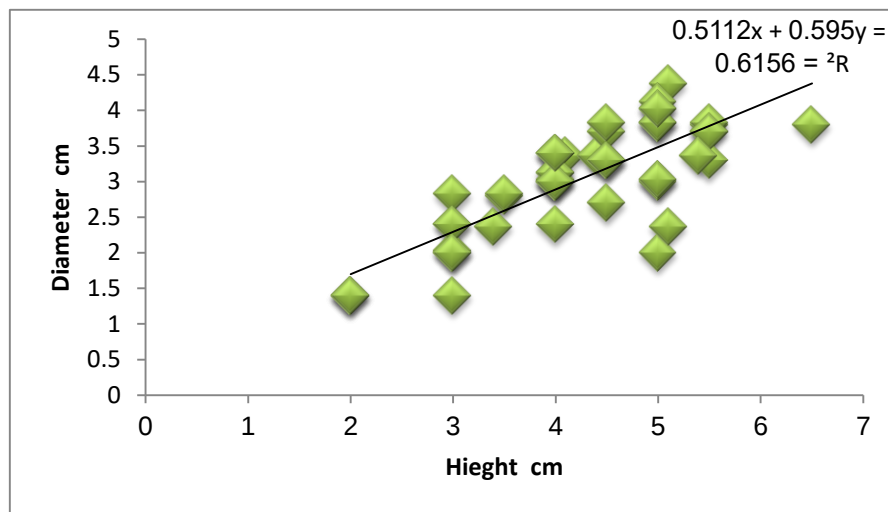


Figure (3): The relationships between height, diameter and size index

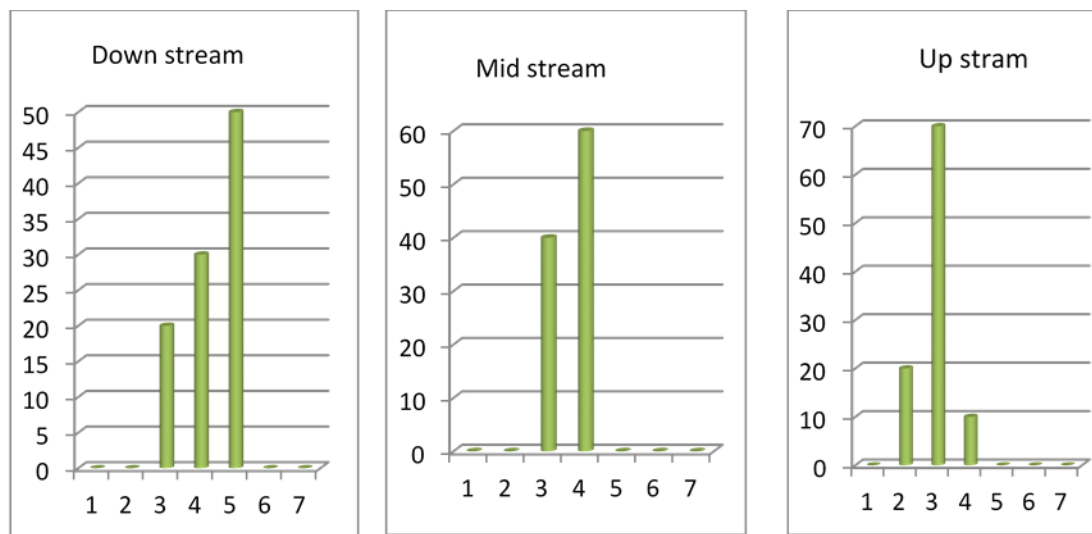


Figure (4): Size frequency distribution of *Laurus nobilis* populations. The ranges of size classes are: 1>1 , 2=1.1-2, 3=2.1-3 ,4=3.1-4 ,5=4.1-5, 6=5.1-6, 7=6.1-7.

Table (1): Size distribution analysis of *Laurus nobilis* population (H: Height, D: Diameter, r: simple linear correlation coefficient between height and diameter and size index)

Sites	Species	H (m)	D (m)	H/D	r ²	Size index (m)
Downstream	<i>Laurus nobilis</i> L.	5.5 ± 0.844	2.1 ± 0.255	2.6 ± 0.532	0.616	5.32 ± 0.811
Midstream	<i>Laurus nobilis</i> L.	4.6 ± 0.721	2.2 ± 0.255	2 ± 0.322	0.616	4.56 ± 0.723
Upstream	<i>Laurus nobilis</i> L.	3.4 ± 0.511	2.5 ± 0.361	1.4 ± 0.111	0.616	3.22 ± 0.577

Table (2): Soil chemical and physical analysis in each of the three habitats recognized in the study area.

Soil variables	Elevation levels			F – value
	Downstream	Midstream	Upstream	
pH value	8.4±0.32	7.5±0.21	7.5±0.22	0.317
E.C ds/m	0.344±0.247	0.144±0.76	0.283±0.236	2.88*
Sand (%)	26.8±3.77	29.55±6.22	33.22±6.11	0.252
Silt (%)	40.1±7.16	37.51±6.3	42.2±9.1	1.95
Clay (%)	37.1±9.52	58.24±11.22	33.6±12.04	2.97*
CO ₃ -m.eq./L.)	0.0±0.0	0.0±0.0	0.0±0.0	0.0
HCO ₃ -(m.eq./L.)	0.75±0.22	0.55±0.64	0.45±0.44	0.112
SO ₄ -(m.eq./L.)	5.22±4.3	1.55±1.32	0.75±2.3	0.832
Cl (m.eq./L.)	0.76±0.12	0.71±1.1	0.94±3.1	1.22
Ca ⁺² (m.eq./L.)	0.51±1.14	0.91±0.44	0.16±0.6	0.163
Mg ⁺² (m.eq./L.)	0.02 ±0.15	0.05±0.88	0.31±0.69	0.362
Na ⁺ (m.eq./L.)	6.6±5.79	3.18±0.46	1.44±1.52	0.944
K ⁺ (m.eq./L.)	0.09±1.99	0.29±0.58	0.33±0.42	0.937

*= significant at P= 0.05

DISCUSSION

Laurus nobilis was observed in three different habitats (upstream, midstream, and downstream) in this study. Its presence was more significant in the first three habitats (downstream), according to the current study. Accordingly, compared to species with smaller morphological variations, those with larger morphological variations would be more adapted to wide environment gradients (Pang & Jiang, 1995). The height-to-diameter ratio provides insight into the plant's growth habit; changes in this ratio are primarily caused by spacing (Wonn & O'Hara, 2001), indicating a tendency for these species' diameters to expand vertically as opposed to horizontally. This ratio in the current study marginally exceeds unity, indicating that people have a tendency to expand (Galal, 2011).

Furthermore, the distribution of *Laurus nobilis* was negatively skewed, suggesting that mature individuals predominate over juvenile ones. Due to the population's high proportion of larger individuals relative to smaller ones), this distribution is indicative of a declining population. Variations in growth rates brought on by age differences, genetic variation, resource heterogeneity, and competition can also contribute to size differences within the plant population (Weiner, 1985). The population's size structure in the wadi beds was close to the distribution's negative skew, suggesting that mature individuals predominated over juvenile ones. Because there are more large individuals in the population than small ones (limited regeneration capacity), this distribution has been associated with declining populations (Weiner, 1984). The study conducted soil analysis at various elevation levels and found that plant cover and vegetation variables were positively correlated with altitude at Shahat. Additionally, soils at elevation downstream had the highest values of sodium, bicarbonate, sulfate, and E.C. The highest concentrations of clay, silt, and chloride were found in mid-stream soils, while the lowest concentrations were found in E.C.

CONCLUSION

In summary, the overall demographic makeup of *Laurus nobilis* populations in the studied region is distinguished by a greater proportion of elderly individuals relative to younger ones. Genetic, environmental, or dominance-and-suppression competition can be sources of discontinuous variation. Because only the smaller plants are negatively impacted by this type of competition, it could be regarded as asymmetric (Abdalrhim, 2021). Since human activity contributes significantly to the worsening of the situation, species may be able to adapt to and survive climate change (Mawdsley *et al.*, 2009).

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

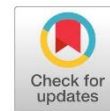
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Assessment of Content Cations Present in Groundwater Samples Collected from Wells of Ajdabya City and its Environs

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Abstract

The purpose of this study was aimed to evaluate the quality of the drinking water in fifteen wells from Ajdabya City and its surrounding areas. By measuring the conductivity, total dissolved solids, major calcium (Ca²⁺), magnesium (Mg²⁺), sodium (Na⁺), potassium (K⁺), lithium (Li⁺), and total hardness (TH) in the groundwater. According to this study, the conductivity, total dissolved solids, and cation concentrations were rose in the majority of the groundwater samples except in forth wall of Zuwaytinah area, which was in limiting value (EC = 770), (TDS = 340), (TH = 360), (Ca²⁺ = 160). Meanwhile rest the chemical analysis were higher than limiting value (Na⁺ = 390), (K⁺ = 60) and (Li⁺ = 60) when compared to the WHO and Libyan drinking water standards.

Keywords: Groundwater; Cations; Flame photometry; Titration; Ajdabya City.

INTRODUCTION

Water is the source of life on Earth for all living organisms, as Allah Almighty says in the Munificent Quran {And, We made from water every living thing} (The Prophets:30). The two main sources of it are surface water and groundwater (Dawood & Sanad, 2014; AZAZA et al., 2012), and about one-third of people on Earth use groundwater for drinking (Nickson et al., 2005). One valuable natural water resource that is suitable for residential use and is easily accessible is groundwater (Najafi et al., 2020). In arid and semiarid regions, groundwater has traditionally been the preferred source of drinking water (Loh et al., 2020). Subterranean water is the world's primary source of drinking water and is also utilized as a backup supply for the industrial and agricultural sectors (Mishra & Bhatt, 2008)). Elements exist in aquatic systems as suspended, colloidal ions, dissolved ions and complexes, and solid in sediments. The ionic strength, pH, redox potential, biological processes, and activities all have a significant impact on the concentrations of these ions (Arjonilla et al., 1994).

Numerous techniques for analyzing ions (anions and cations) in water have been documented in the literature. Water cation analysis has historically been done using flame atomic absorption spectrophotometry (Aberoumand & Deokule, 2009). Flame atomic emission is another name for flame photometry. The study of species in the form of atoms is known as spectrometry, and it primarily relies on the ionization of salts containing alkali metals that are drawn into a non-luminous flame.



When alkali metal salt absorbs enough energy from a flame, it vaporizes and emits light with a distinctive wavelength that can be seen by a change in color intensity (Chikhale & Chikhale, 2017).

The present study aims to evaluate a simple, fast, and accurate method for the determination of pH, electrical conductivity, and cations, which included (total hardness, calcium ion, magnesium ion, sodium ion, and potassium ion) in different sites of wells water samples of groundwater, which collected in the year 2019 from Ajdabya City in Libya and its Environs.

MATERIALS AND METHODS

Sample Collection:

In this study, fifteen groundwater samples were taken from three different areas in Ajdabya City and its surroundings: The Sultan and Zuwaytinah areas. Five samples from various well sites were taken from each locality. 500 ml plastic bottles were used to collect the samples. The water samples were later brought to the lab. A water quality parameter test was conducted right away. After that, nitric acid was added to the models in order to preserve the metal content for as long as possible during storage.

Materials

Sodium Hydroxide (NaOH) Guangdong, 515021, China. Ammonia chloride (NH₄Cl) Riedel-DeHaen Germany. Ethylenediaminetetraaceticdisodium (EDTA₂Na) Riedel-DeHaen Germany. Ammonia NH₃. Deionized water was used for preparation of solutions. And the reagents which used are Powder Eriochrome Black T and powder murexide MERK company Germany.

Electrical Conductivity and Total Dissolved Solids:

The conductivity and TDS measurements were carried out using (Conductivity / Temp / TDS meter Goldpoint Company Ltd (Taiwan)). Then, the samples were measured when the laboratory was reached, and stabilize the sample temperature at 25.

Determination of Total Hardness

The total hardness (TH) was measured by the Lind method, in this method we took 5-10ml of the groundwater sample, then the volume was completed with distilled water to 50ml and titrated with (Na₂EDTA) solution 0.01N after raising the pH of the sample solution to 10 by adding 1ml of ammonia regulator solution. Then add a suitable amount of Erichrom Black-T powder as a dry indicator until the color changes to blue. Then we took the average of the reading. [10] The total hardness is calculated according to the following equation:

$$\text{Total Hardness} = \frac{V_{\text{Na2EDTA}} \times N_{\text{Na2EDTA}} \times 1000 \times \text{M.W as CaCO}_3}{V_{\text{sample}}}$$

Determination of Calcium ion:

Calcium ion was calculated by taking 5-10ml of the filtered groundwater sample and then softening the complete volume with distilled water to 50 ml in a correction method using the standard solution (Na₂EDTA) 0.01N, then the pH raised to 13-14 by adding 2ml of NaOH 0.1N and used the Murexid as a dry powder 0.2 g indicator to change the color to solid blue (APHA, 1926). Calcium ions calculated according to the following equation:

$$\text{Calcium Hardness} = \frac{V_{\text{Na2EDTA}} \times N_{\text{Na2EDTA}} \times 1000 \times \text{M.W as CaCO}_3}{V_{\text{Sample}}}$$

Determination of Magnesium ion:

Magnesium ion was estimated by the difference between total hardness and hardness of calcium as expressed in the following equation:

$$\text{Magnesium hardness Mg (mg / L)} = \text{Total hardness CaCO}_3 \text{ (mg/L)} - \text{Calcium hardness (mg / L)}$$

Determination of ions (Na^+ , K^+ , Ba^{+2} and Li^+):

The Concentrations of different ions (Na^+ , K^+ , Ba^{+2} , and Li^+) were measured using flame photometer equipment. The device depends on the Flame Photo Meter on a solution containing metal ions in the flame.

RESULTS

The chemical parameters measured to electrical conductivity, total dissolved solids and some cations from groundwater wells were precisely analyzed and compared with the regulatory standards set by the World Health Organization and Libyan Standards Specification. According to the amount the cations Na^+ , and K^+ were measured using Flame Photometer. Whereas Ca^{2+} , Mg^{2+} , and total hardness which determined by titration methods. The results reveal that the mean values of cation concentrations in groundwater samples studies were quite variable which are illustrated in Tables (1-6). From the results, that illustrated in Table 1, the conductivity and total dissolved solids of well samples in Ajdabya City were not within the allowable limit to Libya Standard Specification NO.82 for drinking water (750 -1200) (500-1000), all of which have high values (1309- 2810) (1083-1570). As noted in Table 2 the conductivity and total dissolved solids of wells water samples in the Zuwaytinah area were higher than the permissible limit. Except in well NO. 4, which the conductivity average and total dissolved solids values are approximately 770 mg/L and 340 mg/L respectively. Table 3 shows the conductivity and total dissolved solids of wells water samples in the Sultan area were very high values (3390-1361) (2243- 1077).

Table 1: The analytical results of wells water samples for conductivity and total dissolved solids (mg/L) in Ajdabya City.

Well site	1	2	3	4	5
EC	2810 $\pm$ 0.153	1309 $\pm$ 0.0743	1487 $\pm$ 0.0653	1438 $\pm$ 0.0272	1979 $\pm$ 0.0840
TDS	1570 $\pm$ 0.0048	1083 $\pm$ 0.0574	1284 $\pm$ 0.0761	1103 $\pm$ 0.0032	1489 $\pm$ 0.0659

Mean $\pm$ SD

Table 2: The analytical results of wells water samples for conductivity and total dissolved solids (mg/L) in Zuwaytinah area.

Well site	1	2	3	4	5
EC	1530 $\pm$ 0.077	1155 $\pm$ 0.603	1430 $\pm$ 0.541	770 $\pm$ 0.0967	3530 $\pm$ 2.0455
TDS	1150 $\pm$ 0.073	1030 $\pm$ 0.037	1109 $\pm$ 0.033	340 $\pm$ 0.0043	1993 $\pm$ 0.0436

Mean $\pm$ SD

Table 3: The analytical results of wells water samples for conductivity and total dissolved solids (mg/L) in Sultan area.

Well site	1	2	3	4	5
EC	3256 $\pm$ 1.069	2690 $\pm$ 0.322	3390 $\pm$ 2.851	1876 $\pm$ 0.0438	1361 $\pm$ 0.0711
TDS	1860 $\pm$ 0.055	1498 $\pm$ 0.0908	2243 $\pm$ 0.377	1366 $\pm$ 0.0421	1077 $\pm$ 0.033

Mean $\pm$ SD

The maximum concentrations of total hardness of wells water samples in Table 4 at Ajdabya City were not within the allowable limit according to Libya Standard Specification NO.82 for drinking water (200-500 mg/L). Except for groundwater samples of well site NO. 2, the amount of water

hardness was nearly 450 mg/L, which was match of the allowable limit. Table 5 recorded the amount of total hardness of wells water samples in the Zuwaytinah area was higher than the permissible limit. Except in wells NO. 2 and 4 which were average of total hardness values approximately 472 mg/L and 380 mg/L respectively.

Table 6 also showed the concentration of water hardness in the Sultan area's well samples, all of which were found to be over the allowable limit. Variations in the amount of heavy rain, leachate drainage from agricultural fields, and the use of well water for farming and gardening all had an impact on the total hydrocarbon (TH) content of groundwater. Water samples are classified as soft ($>1-70$ mg/L), moderately hard (75–150 mg/L), hard (150–300 mg/L), and extremely hard (> 300 mg/L) based on TH (Boyd, 2003). The groundwater wells under analysis had levels of lead above the permissible 500 mg/L drinking water limit. The water samples were deemed excessively hard and not fit for domestic use or consumption. Table 7 shows the comparison of the Libya standard NO.82 limits for Cations in water with WHO limits (mg/L).

Table 4: The analytical results of wells water samples for cations concentration (mg/L) in Ajdabya City.

Well site	TH	Ca	Mg	Na	K	Li
1	1226 $\pm$ 0.588	812 $\pm$ 0.011	414 $\pm$ 0.009	390 $\pm$ 0.965	60 $\pm$ 0.003	10 $\pm$ 0.007
2	450 $\pm$ 0.065	226 $\pm$ 0.022	224 $\pm$ 0.0744	230 $\pm$ 0.005	10 $\pm$ 0.011	10 $\pm$ 0.0322
3	592 $\pm$ 0.081	320 $\pm$ 1.012	272 $\pm$ 0.090	320 $\pm$ 0.076	200 $\pm$ 0.015	30 $\pm$ 0.099
4	632 $\pm$ 0.172	360 $\pm$ 0.0134	272 $\pm$ 0.011	280 $\pm$ 0.524	20 $\pm$ 0.006	30 $\pm$ 0.0322
5	773 $\pm$ 0.987	426 $\pm$ 0.832	347 $\pm$ 0.004	340 $\pm$ 0.099	20 $\pm$ 0.0943	20 $\pm$ 0.066

Mean $\pm$ SD. TH = Total Hardness

Table 5: The analytical results of wells water samples for cations concentration (mg/L) in Zuwaytinah area.

Well site	TH	Ca	Mg	Na	K	Li
1	747 $\pm$ 0.0867	162 $\pm$ 0.0944	585 $\pm$ 0.0521	720 $\pm$ 0.0965	100 $\pm$ 1.094	60 $\pm$ 0.0063
2	472 $\pm$ 0.076	226 $\pm$ 0.073	246 $\pm$ 0.098	430 $\pm$ 0.134	90 $\pm$ 0.055	60 $\pm$ 0.0433
3	735 $\pm$ 0.0023	226 $\pm$ 0.986	509 $\pm$ 0.0547	570 $\pm$ 0.861	80 $\pm$ 0.997	60 $\pm$ 0.033
4	380 $\pm$ 0.943	160 $\pm$ 1.009	220 $\pm$ 0.022	390 $\pm$ 0.654	60 $\pm$ 1.066	60 $\pm$ 0.643
5	3448 $\pm$ 2.985	746 $\pm$ 0.873	2702 $\pm$ 0.512	4050 $\pm$ 0.032	300 $\pm$ 0.009	300 $\pm$ 0.055

Mean $\pm$ SD. TH = Total Hardness

Table 6: The analytical results of wells water samples for cations concentration (mg/L) in Sultan area.

Well site	TH	Ca	Mg	Na	K	Li
1	1853 $\pm$ 0.044	426 $\pm$ 0.0941	1427 $\pm$ 0.991	3500 $\pm$ 2.054	200 $\pm$ 0.006	200 $\pm$ 0.031
2	1226 $\pm$ 0.0376	240 $\pm$ 0.33	986 $\pm$ 0.721	600 $\pm$ 0.0766	240 $\pm$ 0.741	60 $\pm$ 0.132
3	3228 $\pm$ 1.381	692 $\pm$ 0.806	2536 $\pm$ 1.873	7150 $\pm$ 2.965	350 $\pm$ 0.0464	80 $\pm$ 0.0877
4	772 $\pm$ 0.055	226 $\pm$ 0.070	546 $\pm$ 0.543	640 $\pm$ 0.135	40 $\pm$ 0.733	30 $\pm$ 0.125
5	720 $\pm$ 0.0041	182 $\pm$ 0.866	538 $\pm$ 0.114	510 $\pm$ 0.955	40 $\pm$ 0.883	30 $\pm$ 0.667

Mean $\pm$ SD. TH = Total Hardness

Table 7: Comparison of the Libya standard NO.82 limits for Cations in water with WHO limits (mg/L).

Major Ion	Libya standard NO.82 (mg/L)	WHO limit (mg/L)
TDS	500-1000	1000
TH	200-500	500
Ca ²⁺	75-200	200
Mg ²⁺	30-150	150
Na ⁺	20-200	200
K ⁺	10-40	100
Li ⁺	0-0.7	-

DISCUSSION

(812 mg/L). In addition, the present data illustrated that the lowest concentration of Ca²⁺ was found in wells NO. 1 and 4 of the Zuwaytinah area which were 162 mg/L and 160 mg/L respectively. While the other wells were not within the permissible limit. Whereas Ca²⁺ values in the Sultan area as shown in Table 6 find that all wells were not within the permissible limit, except well NO. 5 Ca²⁺ amount was within the permissible limit which was approximately 182 mg/L. The abundance of Ca²⁺ in water is mostly due to its usual presence in Earth's crust (Deshpande et al., 2012). Most of the groundwater wells had a high distribution of Ca²⁺, exceeding the WHO-recommended limit for drinking water (WHO, 2004). The main water chemistry of the groundwater wells may reflect the geology of the area. The total concentration of Ca²⁺ is the main factor that increases the hardness of water (Sadat-Noori et al., 2014). According to study results of magnesium concentration of wells water samples in Ajdabya City, note that all readings were higher than the permissible limit which is (30 mg/L -150 mg/L). Where the reading of the analytical results is nearly (224mg/L-414 mg/L). The highest values of magnesium ions in the Zuwaytinah area, which ranging 220mg/L to 2702mg/L. In addition, the present data illustrated that the highest concentration of Mg²⁺ in the Sultan area was found in all wells, which were nearly from 538 mg/L to 2536mg/L. The abundance of Mg²⁺ in the groundwater wells referred to the dissolution of all solids and rocks but mostly from limestone, dolomite, and gypsum, which are found in large quantities in some brines (Basem et al., 2010; Chenini et al., 2010).

Sultan area of all wells water samples were above of permitted limit which ranging from (20mg/L – 200mg/L). The presented information shows that potassium ion concentration in all wells water samples of Ajdabya City was within the permissible limit which is (10mg/L – 40mg/L). except in well NO. 1 the result obtained was nearly 60mg/L which overtook permissible limit. According to the results obtained in the present work, the K⁺ content in the Zuwaytinah area was not within permissible limits in all wells water samples. Whereas, found that the amount of K⁺ of both wells NO. 4 and 5 in of Sultan area which were within the permitted limit. while the highest average values of K⁺ content were found in wells NO. 1, 2, and 3 which outran the permitted limit. Potassium may primarily come from rock weathering in addition to solid and liquid wastes (Tikle et al., 2012; Belkhiri & Narany, 2015).

Tables delineate that Li⁺ concentration in Ajdabya City, Zuwaytinah area, and Sultan area of all wells water samples was above the permitted limit which ranging from (0 mg/L – 0.7 mg/L). Groundwater is a major source of freshwater in the Arab world, and in most cases, fresh groundwater originates from leakage and vertical precipitation of fresh rainwater, rivers, and lakes through cracks, fractures, and sedimentary rock layers into the aquifer. Groundwater is saltier than surface

water, salt concentrations may be higher than some of the taste, color, and hardness of the water below the surface of the earth, whether in saturated areas is the area filled with their water, or unsaturated which are directly below the surface of the earth and contain geological materials that makeup water and air in the spaces between the soil granules. Ions seeped out of rocks and soils and dissolved in water as a result of weathering and water circulation. The main elements affecting the geochemistry of the water are the geological formations, the water-rock interaction, and the relative mobility of ions (Yousef et al., 2009). It is important to consider major ions and their ratios when attempting to deduce how rock chemistry affects water composition (Shaltami et al., 2017).

CONCLUSION

In summary, most the results obtained in this study was higher than the Libya standard and WHO limit. Groundwater is saltier than surface water, salt concentrations may be higher than area to another. That are primarily come from rock nature in addition to solid and liquid wastes.

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

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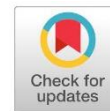
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Research Article

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Synthesis, Characterization (I.R, Elemental analysis, Molar Conductivity), and Antibacterial Investigation of Complex produced by the reaction between Co (II) ion with mixed ligands of (Amoxicillin and Salen)

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Abstract

The complex of cobalt (II) was prepared with the mixed ligand (amoxicillin and salen), and the formed complex was characterized using infrared (I.R.) spectroscopy, elemental analysis of (C%, H%, N%, and M%), molar conductivity methods, and melting point to characterize the complex. The results indicated that the complex is relatively insoluble in aqueous solutions and has significant antibiotic activity against colon bacteria. They also showed that the mixed complex formed has an octahedral structure and has a good electrolytic nature.

Keywords: Amoxicillin- Salen, Co complex, Infrared spectra, antibiotic.

INTRODUCTION

Metal complexes of drugs have changed many of the toxicological, pharmacological, physical, and chemical properties of those drugs (Wu et al., 2003). Dosage forms and drug distribution are strongly tied to a medication's physicochemical properties, and these properties are influenced by the complex formation mechanism in one way or another, which may be beneficial or maybe the opposite. These properties include the complex's solubility, energy absorption, stability, and chemical reaction mechanics (Nogueira Silva et al., 2008; Eze et al., 2014). Some studies have shown that the dissolution of some compounds is faster and the bioavailability is greater than that of the physical mixture, and it has been found that the processing properties such as physical state, flow ability, stability, etc. for complexes are better than those of free drugs (Marcolino et al., 2011).



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Numerous metallic drug complexes were created to increase their potency, and after they had undergone a few successful clinical trials, they were analyzed and evaluated. (Mustapha et al., 2014) Amoxicillin is a β -lactam antibiotic that inhibits carboxypeptidase and transpeptidase enzymes, preventing the synthesis of peptidoglycan. Amoxicillin's bio-functional activity, like that of other penicillin, is based on the β -lactam ring (Hrioua et al., 2021). Blocking the activity of beta-lactamases, which are produced by certain bacteria, is currently the most advanced approach. These enzymes make the bacteria resistant to beta-lactam antibiotics. Metallic particles have gained a lot of attention due to their high surface-area-to-volume ratio and usefulness in biological applications. (Khatoon et al., 2017; Khatoon et al., 2018). Amoxicillin is a drug with a molecular weight of $419.45 \text{ gm.mole}^{-1}$ and the chemical formula $\text{C}_{16}\text{H}_{19}\text{N}_3\text{O}_5\text{S} \cdot 3\text{H}_2\text{O}$. It is a crystalline powder that is an almost white or off-white powder that is only moderately soluble in alcohols like methanol ethanol and water (Martindale, 2009). Its UV maximum wavelength (λ_{max}) is 229,272 nm in 0.1N HCl and 230,274 nm in ethanol (O'Neil & Budavari, 2006). Amoxicillin complexes were synthesized with Ni (II), Cu (II), Zn (II), and Ag (I) ions and analyzed using C, H, and N elemental analysis as well as IR spectroscopy. The complexes exhibited enhanced biological activity for the drug (Imran et al., 2006).

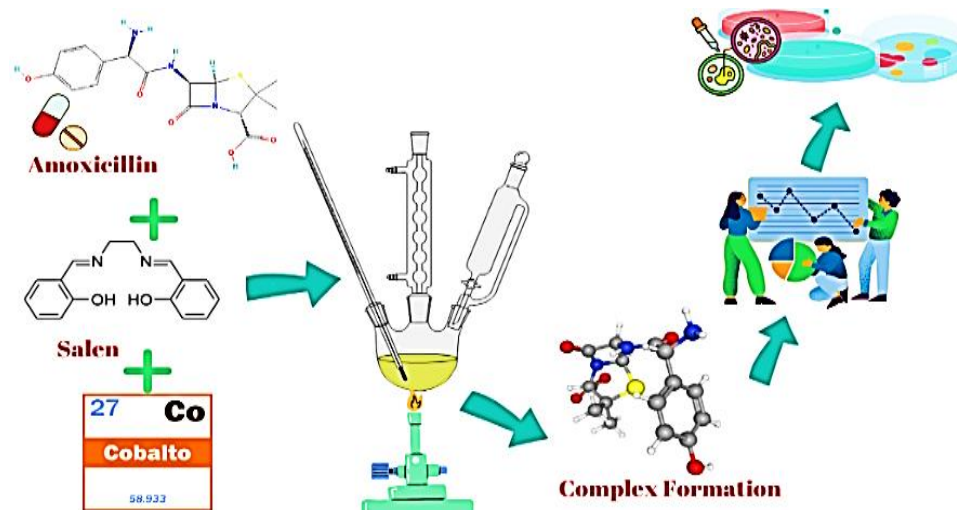


Fig (1). Graphical Abstract

In many kinds of literature, the efficacy of amoxicillin metallic complexes has been discussed (Abou-Hussein & Linert, 2014; Chohan et al., 2004). Studies conducted on the metal complexes of amoxicillin showed that it has great physiological and pharmacological importance, as the drug complexes are stronger than the drugs themselves (Anaconda et al., 2002). The stability of complexes in aqueous and non-aqueous solutions has been investigated using a variety of physical and chemical approaches, such as spectroscopic methods (Ravichandran et al., 2014), potentiometric methods (Sonkamble, 2014), and methods of measuring conductivity (Rezayi et al., 2011). In a previous study, researchers synthesized several complexes of amoxicillin with some transition metals. These complexes were analyzed using elemental analysis, IR, and mass spectra. The stability constant (K_f) of these chelates fell within the range of 10^{-7} to 10^{-14} , and the molar ratio of the complexes was found to be Metal: Drug = 1:1, 1:2. (Zayed & Abdallah, 2005). In a recent study, mixed complexes of the β -lactam antibiotics ampicillin, amoxicillin, and cephalexin were prepared using solutions containing Co (II) and glycine anions (Gly). These complexes, named [Co Gly Ampicillin, Co Gly Amoxicillin, and Co Gly Cephalexin], were analyzed by pH-metric titration at 20°C in an alkaline medium. (Alekseev & Samuilova, 2008). Salen is very important as a ligand as it easily binds to metal ions, forming complexes of various geometries due to the N_2 and O_2 donor

sites it contains. (Clarke & Storr, 2014; Atwood & Harvey, 2001). This study was aimed to synthesis, characterization (I.R, Elemental analysis, Molar Conductivity), and antibacterial investigation of complex produced by the reaction between Co (II) ion with mixed ligands of (Amoxicillin and Salen).

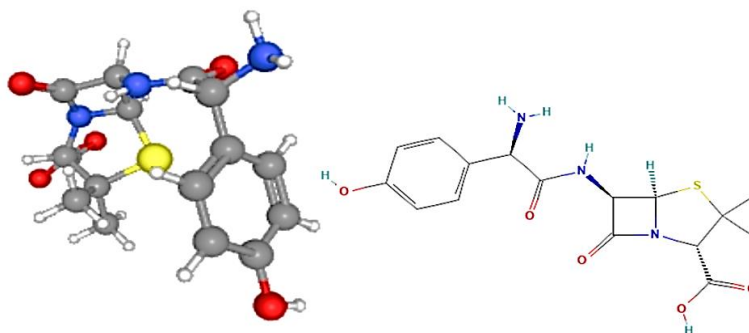


Fig 2: Chemical structure of amoxicillin (AMX)

MATERIALS AND METHODS

Amoxicillin-containing antibiotics were bought from commercial sources. 500 mg of amoxicillin capsules. Other chemicals used in this study are analytical-grade reagents and high purity from Fluka company. All buffer solutions from Sigma–Aldrich.

Synthesis of Salen ligand

To prepare Salen, 0.601 g (0.01 mol) of ethylene diamine and 2.44 g (0.02 mol) of salicylaldehyde were mixed in 50 ml of ethanol. The resulting mixture was re-condensed for 60 minutes. The red crystals formed were isolated by filtration. The crystals were then washed with ethanol and dried at room temperature in a dark place (Tsumaki, 1938).

Synthesis of the Metal-AMX Complexes

A solution of 25 ml methanol was used to dissolve 3 mmol of amoxicillin, followed by adding a solution containing 1 mmol of Co (II) metal chloride in 25 ml of methanol. The ligand was added in a 1:1:1 mole ratio, and the pH was adjusted to 8–9 by adding 1 M methanolic ammonia solution. The mixture was heated at 60–70 °C with constant stirring for about 2 hours. It was then left overnight, filtered, and washed with residual anhydrous calcium chloride and methanol. The collected yield was 62.7% (Refat et al., 2014; Bufarwa & Abdel-Latif, 2022).

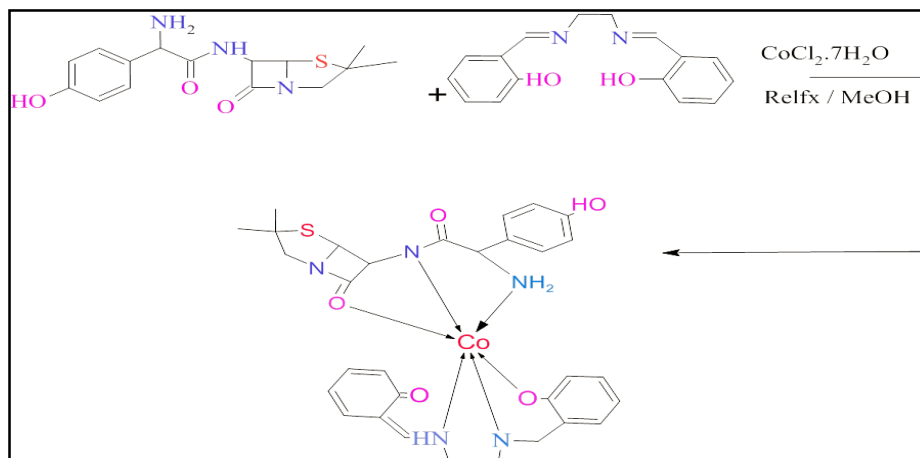


Fig 3: Preparation of [Co (AMX)(S)]

Molar Conductance

The conductivity of a 10^{-3} M complex solution in DMF was measured on a model HACH meter to determine its molar conductance.

Melting point measurements

To determine the melting points of the complex, we used the Stuart Scientific electrothermal melting point apparatus with glass capillary tubes in Celsius degrees.

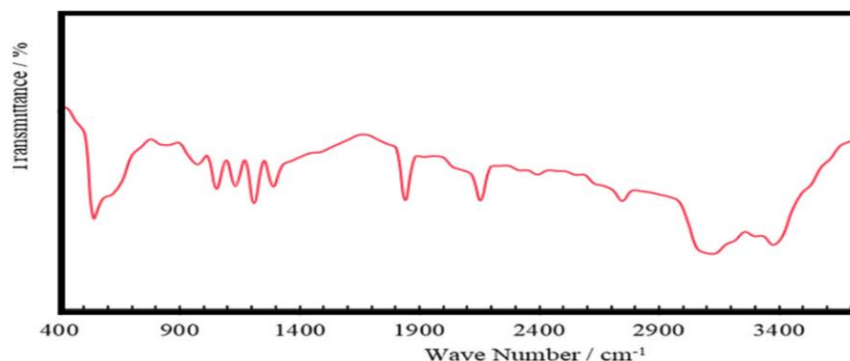


Fig 4: FT-IR of [Co(AMX)(S)]

RESULTS AND DISCUSSION

Elemental analysis of the solid complex was conducted to compare the calculated and found values for carbon, hydrogen, and nitrogen. Table 1 shows the obtained elemental analysis values. Conductivity measurement of the prepared complex also revealed that chloride ions are present outside the coordination sphere.

Table 1: The proposed formula, color, melting point, conductivity, and elemental analysis of the complex

Compound	M. wt. (g/mol)	Yield %	Color	Conduc- tivity μ S	M.P	Anal. Calc. (Found)%			
						N	H	C	Co
[Co (AMX)(S)] C ₃₁ H ₃₇ CoN ₅ O ₅ S	650.65	62.7	Red	121	248	54.75 (57.22)	5.38 (5.73)	9.88 (10.76)	8.52 (9.06)

FT-IR spectra: Studying the infrared spectrum is very important to determine the status of the chelation process as well as the location of coordination. Figure 3 shows the FT-IR spectra of the mixed complex of amoxicillin (AMX) and salen (S) with the cobalt (II) ion. At 1400cm^{-1} , the benzene ring's stretching vibration band $\nu(\text{C}=\text{C})$ is exhibited (Hrioua *et al.*, 2021). While the bands of the hydroxyl and ammonium groups still appear unchanged, as they have not undergone any displacement because they did not enter as ligands in the formation of the complex (Gasheva *et al.*, 1984). The stretching and vibration bands between metal ions and oxygen of the carbonyl group are responsible for the occurrence of bands at $500\text{-}600\text{ cm}^{-1}$. Similarly, the vibration bands between amino groups and metal ions are classified as $\nu(\text{M-N})$ stretching bands between 400 and 500 cm^{-1} (Reiss *et al.*, 2015). The distinctive band at about 3300 cm^{-1} indicates the presence of water molecules outside the coordination sphere in AMX complexes.

Antibacterial activity

The disk diffusion method has been used to examine the antibacterial effectiveness of the cobalt complexes (AMX.S) against *E. coli* (Bonev *et al.*, 2008). The type of the metal ion and the chelate stability are likely to be blamed for the antibacterial action of AMX-salen complexes (Hrioua *et al.*, 2021). Antibiotics made of metal complexes are very effective against resistant strains. Due to their potential to affect drug-induced metallo-enzyme inhibition, cobalt ions remain an area of interest in bioinorganic research for their impact on pathogens, influenza, cancers, and inflammation (Saleh *et al.*, 2023).

Table 2: Inhibitor zone of antibacterial by different concentrations of complex

Concentration µg/L	Inhibitor zone diameter (in mm)	
	AMX	[Co(AMX)(S)]
10	-	10.76
25	-	15.68
50	12.4	19.43

CONCLUSION

The mixed amoxicillin ligands were studied in the form of capsules and the salen ligand with the cobalt binary ion, and some properties were studied to confirm the formation of a complex of mixed ligands of this type. The results showed that the complex formed has an octahedral form, and is an electrolyte in nature because the two chloride atoms are outside the coordination sphere of the complex, and are stable under normal conditions. It was observed that as the concentration of the complex increased, its effectiveness against *E. coli* bacteria increased.

Duality of interest: The authors declare that they have no duality of interest associated with this manuscript.

Author contributions: Contribution is equal between authors.

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