# OF COMPUTER 

 SCIENCELVIII

Yerevan
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PROBLEMS

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Институт проблем информатики и автоматизации Национальной академии наук Республики Армения

Institute for Informatics and Automation Problems of the National Academy of Sciences of the Republic of Armenia

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## Математические проблемы компьютерных наук

## Mathematical Problems of Computer Science

## LVIII

#   <br> ОПУБЛИКОВАНО ИНСТИТУТОМ ПРОБЛЕМ ИНФОРМАТИКИ И АВТОМАТИЗАЦИИ НАН РА <br> PUBLISHED BY INSTITUTE FOR INFORMATICS AND AUTOMATION PROBLEMS OF NAS RA 

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ISSN 2579-2784 (Print)
ISSN 2738-2788 (Online)
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## Математические проблемы компьютерных наук, LVIII

Журнал Математические проблемы компьютерных наук издается два раза в год Институтом проблем информатики и автоматизации НАН РА. Он охватывает современные направления теоретической и прикладной математики, информатики и вычислительной техники.

Он включен в список допустимых журналов Высшей квалификационной комиссии.
Печатается на основании решения $\mathrm{N} 22-11 / 2$ заседания Редакционного совета от 25 ноября 2022г.

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ISSN 2579-2784 (Print)
ISSN 2738-2788 (Online)
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The periodical Mathematical Problems of Computer Science is published twice per year by the Institute for Informatics and Automation Problems of NAS RA. It covers modern directions of theoretical and applied mathematics, informatics and computer science.

It is included in the list of acceptable journals of the Higher Qualification Committee.

Printed on the basis of decision N 22-11/2 of session of the Editorial Council dated November 25, 2022.

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ISSN 2579-2784 (Print)
ISSN 2738-2788 (Online)
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# Analytical Inversion of Tridiagonal Hermitian Matrices 

Yuri R. Hakopian and Avetik H. Manukyan<br>Yerevan State University, Yerevan, Armenia<br>e-mail: yuri.hakopian@ysu.am, avetiq.manukyan1@ysumail.am


#### Abstract

In this paper we give an algorithm for inverting complex tridiagonal Hermitian matrices with optimal computational efforts. For matrices of a special form and, in particular, for Toeplitz matrices, the derived formulas lead to closed-form expressions for the elements of inverse matrices. Keywords: Inverse matrix, Tridiagonal matrix, Hermitian matrix, Toeplitz matrix. Article info: Received 21 April 2022; received in revised form 15 July 2022; accepted 23 August 2022.


## 1. Introduction

Tridiagonal matrices are encountered in many areas of applied mathematics. Such matrices are of great importance in finite difference and finite element methods for differential equations. The construction of cubic splines is reduced to solving systems with tridiagonal matrices. Symmetric matrices are reduced to tridiagonal matrices by the similarity Householder transformation (see [1, 2, 3], for instance). Other examples can be cited.

There is a well-known fast numerical method for solving systems with tridiagonal matrices. At the same time, the analytical matrix inversion is also of certain interest (see $[4,5,6]$, for instance). For tridiagonal matrices of special types, this leads to closed-form expressions for the elements of inverse matrices $[7,8,9,10]$. This is undoubtedly useful in theoretical considerations. Further, explicit formulas can be a part of more general computational procedures. There are other reasons as well.

In this article, we focus our attention on complex Hermitian tridiagonal matrices. We will construct a fairly simple computational procedure, consisting of a sequence of recurrence relations, leading to the calculation of the elements of the inverse matrix. In special cases, in particular for Toeplitz tridiagonal Hermitian matrices, the procedure can become the basis for deriving closed-form expressions for the elements of the inverse matrix.

We note right away that throughout this article $\bar{z}$ stands for the complex conjugate of the complex number $z$.

Let a nonsingular tridiagonal Hermitian matrix

$$
A=\left[\begin{array}{ccccc}
a_{1} & b_{1} & & &  \tag{1}\\
\overline{b_{1}} & a_{2} & b_{2} & & 0 \\
& \ddots & \ddots & \ddots & \\
0 & & \overline{b_{n-2}} & \frac{a_{n-1}}{b_{n-1}} & b_{n-1} \\
& & & a_{n}
\end{array}\right]
$$

be given, where $a_{i}, i=1,2, \ldots, n$ are real numbers and $b_{i} \neq 0$ for $i=1,2, \ldots, n-1$. In accordance with the accepted notation, $A=A^{*}$. We assume that $n>3$. The requirement that the subdiagonal (superdiagonal) elements of the matrix be nonzero is not restrictive. Indeed, if some of these elements are equal to zero, the problem of computing the inverse matrix is decomposed into several similar problems for tridiagonal matrices of lower order.

## 2. Preliminary Calculations

Let $A^{-1}=\left[x_{i j}\right]_{n \times n}$. This matrix is also Hermitian. In our considerations we will use the notation

$$
X^{(j)} \equiv\left[x_{1 j} x_{2 j} \ldots x_{n j}\right]^{T}, \quad j=1,2, \ldots, n
$$

for the columns of the inverse matrix.
The matrix A can be represented as a product

$$
\begin{equation*}
A=D B \tag{2}
\end{equation*}
$$

of the matrices

$$
\begin{equation*}
D=\operatorname{diag}\left[b_{1}, \overline{b_{1}}, \overline{b_{2}}, \ldots, \overline{b_{n-2}}, \overline{b_{n-1}}\right] \tag{3}
\end{equation*}
$$

and

$$
B=\left[\begin{array}{cccccc}
p & 1 & & & &  \tag{4}\\
1 & f_{2} & g_{2} & & 0 & \\
& 1 & f_{3} & g_{3} & & \\
& & \ddots & \ddots & \ddots & \\
& 0 & & 1 & f_{n-1} & g_{n-1} \\
& & & & 1 & q
\end{array}\right]
$$

where

$$
\begin{equation*}
f_{i}=\frac{a_{i}}{\overline{b_{i-1}}}, g_{i}=\frac{b_{i}}{\overline{b_{i-1}}}, i=2,3, \ldots, n-1 ; p=\frac{a_{1}}{b_{1}}, q=\frac{a_{n}}{\overline{b_{n-1}}} . \tag{5}
\end{equation*}
$$

Having a nonsingular matrix $B$ defined in (4), let us consider the following system of linear algebraic equations

$$
\begin{align*}
& p \mu_{1}+\mu_{2}=\alpha \\
& \mu_{i-1}+f_{i} \mu_{i}+g_{i} \mu_{i+1}=0, \quad 2 \leq i \leq n-1  \tag{6}\\
& \mu_{n-1}+q \mu_{n}=0
\end{align*}
$$

where we will set the right-hand side $\alpha$ of the first equation a little later. It is easy to verify that regardless of the choice of $\alpha$, the recursively defined quantities

$$
\begin{align*}
& \mu_{n}=1, \mu_{n-1}=-q \\
& \mu_{i-1}=-f_{i} \mu_{i}-g_{i} \mu_{i+1}, i=n-1, n-2, \ldots, 2 \tag{7}
\end{align*}
$$

satisfy all equations of the system (6), starting with the second one. Then, we choose the quantity $\alpha$ as follows:

$$
\begin{equation*}
\alpha=p \mu_{1}+\mu_{2} . \tag{8}
\end{equation*}
$$

Remark 1 Since, by assumption, the matrix $B$ is nonsingular (it follows from (2)), then $\alpha \neq 0$. Indeed, otherwise we would have obtained that the homogeneous system (6) has a nontrivial solution. Further,

$$
\alpha=\frac{a_{1}}{b_{1}} \mu_{1}+\mu_{2}=\frac{1}{b_{1}}\left(a_{1} \mu_{1}+b_{1} \mu_{2}\right) .
$$

Therefore

$$
a_{1} \mu_{1}+b_{1} \mu_{2} \neq 0
$$

as well.
Thus,

$$
\begin{equation*}
\alpha=b_{1}^{-1} t^{-1}, \tag{9}
\end{equation*}
$$

where

$$
\begin{equation*}
t \equiv\left(a_{1} \mu_{1}+b_{1} \mu_{2}\right)^{-1} \tag{10}
\end{equation*}
$$

Let us introduce the vector

$$
r^{(1)} \equiv\left[\mu_{1} \mu_{2} \ldots \mu_{n}\right]^{T},
$$

the components of which are specified in (7). As follows from (4), (6) and (9),

$$
B r^{(1)}=[\alpha 0 \ldots 0]^{T}=\alpha e^{(1)}=b_{1}^{-1} t^{-1} e^{(1)},
$$

where $e^{(1)} \equiv\left[\begin{array}{lll}1 & \ldots 0\end{array}\right]^{T}$. Further, on the basis of factorization (2) of the matrix $A$, we obtain the equality

$$
\begin{equation*}
A r^{(1)}=D B r^{(1)}=b_{1}^{-1} t^{-1} D e^{(1)}=t^{-1} e^{(1)} ; \tag{11}
\end{equation*}
$$

here we have used the obvious equality $D e^{(1)}=b_{1} e^{(1)}$ (see (3)). The equality (11) allows to compute the first column of the inverse matrix $A^{-1}$. Indeed, from this equality we find that

$$
A^{-1} e^{(1)}=t r^{(1)} .
$$

Since $A^{-1} e^{(1)}=X^{(1)}$, then $X^{(1)}=t r^{(1)}$, or

$$
\begin{equation*}
x_{i 1}=t \mu_{i}, \quad i=1,2, \ldots, n . \tag{12}
\end{equation*}
$$

Thus, we have found the first column of the inverse matrix. Similarly, we can calculate the last column of the matrix $A^{-1}$. For this purpose, let us consider the linear system

$$
\begin{align*}
& p \nu_{1}+\nu_{2}=0 \\
& \nu_{i-1}+f_{i} \nu_{i}+g_{i} \nu_{i+1}=0,2 \leq i \leq n-1  \tag{13}\\
& \nu_{n-1}+q \nu_{n}=\beta
\end{align*}
$$

where we will set the right-hand side $\beta$ of the last equation later. Regardless of the choice of $\beta$, the recursively defined quantities

$$
\begin{align*}
& \nu_{1}=1, \nu_{2}=-p, \\
& \nu_{i+1}=-\frac{1}{g_{i}}\left(\nu_{i-1}+f_{i} \nu_{i}\right), i=2,3, \ldots, n-1 \tag{14}
\end{align*}
$$

satisfy the first $n-1$ equations of the system (13). Then we choose the quantity $\beta$ as follows:

$$
\begin{equation*}
\beta=\nu_{n-1}+q \nu_{n} . \tag{15}
\end{equation*}
$$

Since the matrix $B$ is nonsingular, then $\beta \neq 0$ (see Remark 1). Substituting the expression of the quantity $q$ given in (5) into (15) yields

$$
\beta=\nu_{n-1}+\frac{a_{n}}{\overline{b_{n-1}}} \nu_{n}=\frac{1}{\overline{b_{n-1}}}\left(\overline{b_{n-1}} \nu_{n-1}+a_{n} \nu_{n}\right) .
$$

Thus,

$$
\begin{equation*}
\beta={\overline{b_{n-1}}}^{-1} \theta^{-1} \tag{16}
\end{equation*}
$$

where

$$
\theta \equiv\left(\overline{b_{n-1}} \nu_{n-1}+a_{n} \nu_{n}\right)^{-1} .
$$

Now let us introduce the vector

$$
r^{(n)} \equiv\left[\nu_{1} \nu_{2} \ldots \nu_{n}\right]^{T},
$$

the components of which are specified in (14). From (4), (13) and (16) we find that

$$
B r^{(n)}=[0, \ldots 0 \beta]^{T}=\beta e^{(n)}={\overline{b_{n-1}}}^{-1} \theta^{-1} e^{(n)},
$$

where $e^{(n)} \equiv\left[\begin{array}{lll}0 & \ldots & 1\end{array}\right]^{T}$. Having the factorization (2) of the matrix $A$, we obtain the equality

$$
A r^{(n)}=D B r^{(n)}={\overline{b_{n-1}}}^{-1} \theta^{-1} D e^{(n)}=\theta^{-1} e^{(n)}
$$

From here,

$$
A^{-1} e^{(n)}=\theta r^{(n)}
$$

Since $A^{-1} e^{(n)}=X^{(n)}$, then $X^{(n)}=\theta r^{(n)}$, or

$$
\begin{equation*}
x_{i n}=\theta \nu_{i}, \quad i=1,2, \ldots, n . \tag{17}
\end{equation*}
$$

Let us refine the last expression. From (12), $x_{n 1}=t \mu_{n}=t$. Further, according to (17), $x_{1 n}=\theta \nu_{1}=\theta$. Since $A^{-1}$ is a Hermitian matrix, then $x_{1 n}=\overline{x_{n 1}}$. Consequently, $\theta=\bar{t}$, and we come to the conclusion that

$$
\begin{equation*}
x_{i n}=\bar{t} \nu_{i}, \quad i=1,2, \ldots, n . \tag{18}
\end{equation*}
$$

So, we have found the first and the last columns of the Hermitian matrix $A^{-1}$. These are expressions (12) and (18). Taking into account that $\nu_{1}=1$ and $\mu_{n}=1$, we write these elements in the form of

$$
\begin{equation*}
x_{i 1}=t \mu_{i} \overline{\nu_{1}}, x_{i n}=\bar{t} \overline{\mu_{n}} \nu_{i}, \quad i=1,2, \ldots, n . \tag{19}
\end{equation*}
$$

Moreover, the diagonal elements $x_{11}=t \mu_{1} \overline{\nu_{1}}$ and $x_{n n}=\bar{t} \overline{\mu_{n}} \nu_{n}$ are real numbers. Therefore, we can write $x_{n n}=t \mu_{n} \overline{\nu_{n}}$ as well.

Looking ahead, we say that in the next section we will prove that the quantities

$$
\begin{equation*}
t \mu_{i} \overline{\nu_{i}}, \quad i=2,3, \ldots, n-1 \tag{20}
\end{equation*}
$$

are the remaining diagonal elements of the matrix $A^{-1}$. To do this, here we first establish that the quantities (20) are real numbers (naturally, without assuming that they are somehow related to the matrix $A^{-1}$ ).

Let us introduce into consideration the quantities

$$
\begin{equation*}
R_{i} \equiv b_{i-1}\left(t \mu_{i} \overline{\nu_{i-1}}\right)+\overline{b_{i-1}}\left(t \mu_{i-1} \overline{\nu_{i}}\right), \quad i=2,3, \ldots, n-2 . \tag{21}
\end{equation*}
$$

Lemma 1. The quantity $R_{2}$ is a real number.
Proof. Since $\nu_{1}=1$ and $\nu_{2}=-p$ (see (2.13)), then

$$
R_{2}=t\left(b_{1} \mu_{2} \overline{\nu_{1}}+\overline{b_{1}} \mu_{1} \overline{\nu_{2}}\right)=t b_{1}\left(\mu_{2}-p \mu_{1}\right) .
$$

Further, taking into account the equalities (8) and (9), we get

$$
R_{2}=t b_{1}\left(\alpha-2 p \mu_{1}\right)=t b_{1} \alpha-2 p b_{1}\left(t \mu_{1}\right)=1-2 a_{1}\left(t \mu_{1}\right) .
$$

The quantities $a_{1}$ and $t \mu_{1}$ are real numbers, so $R_{2}$ is also a real number.
Lemma 2. The quantities $R_{i}$ from (21) satisfy the relations

$$
\begin{equation*}
R_{i}=-R_{i-1}-2 a_{i-1}\left(t \mu_{i-1} \overline{\nu_{i-1}}\right), \quad i=3,4, \ldots, n-2 . \tag{22}
\end{equation*}
$$

Proof. From (6) we have the equality

$$
\mu_{i-2}+f_{i-1} \mu_{i-1}+g_{i-1} \mu_{i}=0
$$

Using formulas (5), let us write this equality in the form of

$$
\overline{b_{i-2}} \mu_{i-2}+a_{i-1} \mu_{i-1}+b_{i-1} \mu_{i}=0
$$

Multiplying both parts of the last equality by $t \overline{\nu_{i-1}}$, we get that

$$
\begin{equation*}
b_{i-1}\left(t \mu_{i} \overline{\nu_{i-1}}\right)=-\overline{b_{i-2}}\left(t \mu_{i-2} \overline{\nu_{i-1}}\right)-a_{i-1}\left(t \mu_{i-1} \overline{\overline{\nu_{i-1}}}\right) . \tag{23}
\end{equation*}
$$

Similarly, from (13) we have the equality

$$
\nu_{i-2}+f_{i-1} \nu_{i-1}+g_{i-1} \nu_{i}=0
$$

which can be written as follows:

$$
b_{i-2} \overline{\overline{\nu_{i-2}}}+a_{i-1} \overline{\nu_{i-1}}+\overline{b_{i-1}} \overline{\nu_{i}}=0 .
$$

Multiplying both parts of this equality by $t \mu_{i-1}$ yields

$$
\begin{equation*}
\overline{b_{i-1}}\left(t \mu_{i-1} \overline{\nu_{i}}\right)=-b_{i-2}\left(t \mu_{i-1} \overline{\nu_{i-2}}\right)-a_{i-1}\left(t \mu_{i-1} \overline{\nu_{i-1}}\right) . \tag{24}
\end{equation*}
$$

The relation (22) follows directly from the equalities (23) and (24).
Lemma 3. The quantities $\mu_{i} \overline{\nu_{i}}, \quad i=2,3, \ldots, n-1$ are real numbers.
Proof. Consider first the quantity $t \mu_{2} \overline{\nu_{2}}$. Since $p \mu_{1}+\mu_{2}=\alpha$ and $\nu_{2}=-p$ (see (6) and (14)), then

$$
t \mu_{2} \overline{\nu_{2}}=t\left(p \mu_{1}-\alpha\right) \bar{p}=(p \bar{p})\left(t \mu_{1}\right)-t \alpha \bar{p} .
$$

Further, using the equality (9), we obtain that

$$
t \mu_{2} \overline{\nu_{2}}=(p \bar{p})\left(t \mu_{1}\right)-\frac{\bar{p}}{b_{1}}=(p \bar{p})\left(t \mu_{1}\right)-\frac{a_{1}}{b_{1} \overline{b_{1}}} .
$$

Thus, the quantity $t \mu_{2} \overline{\nu_{2}}$ is a real number.

Next, consider the quantity $t \mu_{3} \overline{\nu_{3}}$. As follows from (6) and (13),

$$
\mu_{3}=-\frac{a_{2}}{b_{2}} \mu_{2}-\frac{\overline{b_{1}}}{\overline{b_{2}}} \mu_{1}, \quad \overline{\nu_{3}}=-\frac{a_{2}}{\overline{b_{2}}} \overline{\nu_{2}}-\frac{b_{1}}{\overline{b_{2}} \overline{\nu_{1}} .}
$$

Proceeding from these equalities, we get that

$$
t \mu_{3} \overline{\nu_{3}}=\frac{1}{b_{2} \overline{b_{2}}}\left[a_{2}^{2}\left(t \mu_{2} \overline{\overline{\nu_{2}}}\right)+b_{1} \overline{b_{1}}\left(t \mu_{1} \overline{\nu_{1}}\right)+a_{2} R_{2}\right]
$$

The quantities $t \mu_{1} \overline{\nu_{1}}$ and $t \mu_{2} \overline{\nu_{2}}$ are real numbers. According to Lemma 1, the quantity $R_{2}$ is also a real number. Therefore, $t \mu_{3} \overline{\nu_{3}}$ is a real number as well.

Further reasoning will be carried out by the method of mathematical induction on $i$. Suppose that for some value of $i$, where $3 \leq i \leq n-2$, it is already known that the quantities $t \mu_{k} \overline{\nu_{k}}, k \leq i$ and $R_{k}, k \leq i-1$ are real numbers. From (6) and (13) we have

$$
\mu_{i+1}=-\frac{a_{i}}{b_{i}} \mu_{i}-\frac{\overline{b_{i-1}}}{b_{i}} \mu_{i-1}, \quad \overline{\overline{\nu_{i+1}}}=-\frac{a_{i}}{\overline{b_{i}}} \overline{\nu_{i}}-\frac{b_{i-1}}{\overline{b_{i}}} \overline{\nu_{i-1}} .
$$

Then

$$
t \mu_{i+1} \overline{\overline{\nu_{i+1}}}=\frac{1}{b_{i} \overline{b_{i}}}\left[a_{i}^{2}\left(t \mu_{i} \overline{\nu_{i}}\right)+b_{i-1} \overline{b_{i-1}}\left(t \mu_{i-1} \overline{\nu_{i-1}}\right)+a_{i} R_{i}\right] .
$$

Hence, by virtue of the assumptions made and taking into account the assertion of Lemma 2 , we arrive at a conclusion that the quantity $t \mu_{i+1} \overline{\nu_{i+1}}$ is a real number.
Remark 2 We have established that the quantities $t \mu_{i} \overline{\nu_{i}}, i=1,2, \ldots, n$ are real numbers. Therefore, $t \mu_{i} \overline{\nu_{i}}=\bar{t} \overline{\mu_{i}} \nu_{i}$.

## 3. The Elements of the Inverse Matrix

Above we obtained the expressions (19) for the elements of the first and the last columns of the inverse matrix, as well as some auxiliary statements. Based on these results, here we derive formulas for the remaining elements of the inverse matrix.

Let $2 \leq j \leq n-1$. We introduce into consideration the vector

$$
\begin{equation*}
r^{(j)} \equiv\left[\bar{t} \overline{\mu_{j}} \nu_{1}, \ldots, \bar{t} \overline{\mu_{j}} \nu_{j-1}, t \mu_{j} \overline{\nu_{j}}, t \mu_{j+1} \overline{\nu_{j}}, \ldots, t \mu_{n} \overline{\nu_{j}}\right]^{T} \tag{25}
\end{equation*}
$$

where the quantities $\mu_{i}$ and $\nu_{i}$ are specified in (7) and (14), respectively. Multiplying the matrix B defined in (4) and the vector $r^{(j)}$ yields

$$
\begin{equation*}
B r^{(j)}=z^{(j)} \tag{26}
\end{equation*}
$$

where the components of the vector

$$
z^{(j)}=\left[z_{1}^{(j)} z_{2}^{(j)} \ldots z_{j-1}^{(j)} \delta_{j} z_{j+1}^{(j)} \ldots z_{n-1}^{(j)} z_{n}^{(j)}\right]^{T}
$$

are calculated as follows:

$$
\begin{aligned}
& z_{1}^{(j)}=\bar{t} \overline{\mu_{j}}\left(p \nu_{1}+\nu_{2}\right), \\
& z_{i}^{(j)}=\bar{t} \overline{\mu_{j}}\left(\nu_{i-1}+f_{i} \nu_{i}+g_{i} \nu_{i+1}\right), \quad 2 \leq i \leq j-1, \\
& \delta_{j}=\bar{t} \overline{\mu_{j}} \nu_{j-1}+f_{j}\left(t \mu_{j} \overline{\nu_{j}}\right)+g_{j}\left(t \mu_{j+1} \overline{\nu_{j}}\right), \\
& z_{i}^{(j)}=t\left(\mu_{i-1}+f_{i} \mu_{i}+g_{i} \mu_{i+1}\right) \overline{\nu_{j}}, \quad j+1 \leq i \leq n-1, \\
& z_{n}^{(j)}=t\left(\mu_{n-1}+q \mu_{n}\right) \overline{\nu_{j}} .
\end{aligned}
$$

Having equations (6) and (13), we conclude that $z_{i}^{(j)}=0$ for $1 \leq i \leq j-1$ and $j+1 \leq i \leq n$. Thus,

$$
\begin{equation*}
z^{(j)}=\left[0 \ldots 0 \delta_{j} 0 \ldots 0\right]^{T}=\delta_{j} e^{(j)} \tag{27}
\end{equation*}
$$

where $e^{(j)}=[0 \ldots 010 \ldots 0]^{T}$ (the unit is located on $j$ th place).
It remains to clarify the quantity $\delta_{j}$. Taking into account Remark 2, we have

$$
\begin{align*}
\delta_{j} & =\bar{t} \overline{\mu_{j}} \nu_{j-1}+f_{j}\left(\bar{t} \overline{\mu_{j}} \nu_{j}\right)+g_{j}\left(t \mu_{j+1} \overline{\nu_{j}}\right)  \tag{28}\\
& =\bar{t} \overline{\mu_{j}}\left(\nu_{j-1}+f_{j} \nu_{j}\right)+g_{j}\left(t \mu_{j+1} \overline{\nu_{j}}\right) .
\end{align*}
$$

Since $\nu_{j-1}+f_{j} \nu_{j}=-g_{j} \nu_{j+1}($ see (13)), then

$$
\begin{equation*}
\delta_{j}=g_{j}\left(t \mu_{j+1} \overline{\nu_{j}}-\bar{t} \overline{\mu_{j}} \nu_{j+1}\right), \quad 2 \leq j \leq n-1 . \tag{29}
\end{equation*}
$$

Let us get one more representation of the quantity $\delta_{j}$. Since $g_{j} \mu_{j+1}=-\mu_{j-1}-f_{j} \mu_{j}$ (see (6)), then from(28) it follows that

$$
\delta_{j}=\bar{t} \overline{\mu_{j}} \nu_{j-1}-t \mu_{j-1} \overline{\nu_{j}}+f_{j}\left(\bar{t} \overline{\mu_{j}} \nu_{j}-t \mu_{j} \overline{\nu_{j}}\right) .
$$

From here, according to Remark 2, we obtain

$$
\begin{equation*}
\delta_{j}=\bar{t} \overline{\mu_{j}} \nu_{j-1}-t \mu_{j-1} \overline{\nu_{j}}, \quad 2 \leq j \leq n-1 . \tag{30}
\end{equation*}
$$

Assuming that $3 \leq j \leq n-1$, we can write the expression (30) in the form of

$$
\delta_{j}=\frac{1}{\overline{g_{j-1}}} \overline{g_{j-1}\left(t \mu_{j} \overline{\nu_{j-1}}-\bar{t} \overline{\mu_{j-1}} \nu_{j}\right)} .
$$

Comparing with the record (29), we arrive at the relation

$$
\begin{equation*}
\delta_{j}=\frac{1}{\overline{g_{j-1}}} \overline{\delta_{j-1}}, \quad 3 \leq j \leq n-1 . \tag{31}
\end{equation*}
$$

Based on the relation (31), one can easily show that

$$
\delta_{j}= \begin{cases}{\overline{b_{j-1}}}^{-1} b_{1} \overline{\delta_{2}}, & \text { if } j \text { is odd }  \tag{32}\\ \overline{b_{j-1}}-1 \overline{b_{1}} \delta_{2}, & \text { if } j \text { is even }\end{cases}
$$

Finally, let us calculate the quantity $\delta_{2}$. According to the representation (30), we have

$$
\begin{align*}
\delta_{2} & =\bar{t} \overline{\mu_{2}} \nu_{1}-t \mu_{1} \overline{\nu_{2}}=\bar{t} \overline{\mu_{2}}+t \mu_{1} \bar{p} \\
& =\bar{t} \overline{\mu_{2}}+\bar{t} \overline{\mu_{1}} \bar{p}=\bar{t}\left(\overline{\mu_{2}}+\bar{p} \overline{\mu_{1}}\right)=\bar{t} \bar{\alpha}={\overline{b_{1}}}^{-1}, \tag{33}
\end{align*}
$$

(see (6) and (9)). Thus, from (32) and (33) we conclude that

$$
\begin{equation*}
\delta_{j}={\overline{b_{j-1}}}^{-1}, \quad j=2,3, \ldots, n-1 \tag{34}
\end{equation*}
$$

Summing up the results, from (27) and (34) we come to the equality

$$
\begin{equation*}
z^{(j)}={\overline{b_{j-1}}}^{-1} e^{(j)} \tag{35}
\end{equation*}
$$

Proceeding from the factorization (2) of the matrix $A$ and using the equalities (26) and (35), we have

$$
A r^{(j)}=D B r^{(j)}=D z^{(j)}={\overline{b_{j-1}}}^{-1} D e^{(j)}=e^{(j)}
$$

(note that $D e^{(j)}=\overline{b_{j-1}} e^{(j)}$, which follows from (3)). Further,

$$
A^{-1} e^{(j)}=r^{(j)}
$$

Since $A^{-1} e^{(j)}=X^{(j)}$, then $X^{(j)}=r^{(j)}$. The components of the vector $r^{(j)}$ are given in (25). Thus,

$$
\begin{equation*}
x_{i j}=\bar{t} \overline{\mu_{j}} \nu_{i}, \quad i=1,2, \ldots, j-1 \quad \text { and } \quad x_{i j}=t \mu_{i} \overline{\nu_{j}}, \quad i=j, j+1, \ldots, n . \tag{36}
\end{equation*}
$$

Combining formulas (36) with those of (12) and (18) yields

$$
x_{i j}=\left\{\begin{array}{l}
\bar{t} \overline{\mu_{j}} \nu_{i}, i=1,2, \ldots, j-1,  \tag{37}\\
t \mu_{i} \overline{\nu_{j}}, i=j, j+1, \ldots, n
\end{array} \quad \text { for } j=1,2, \ldots, n .\right.
$$

Note the following. Since the matrix $A^{-1}$ is also Hermitian, then in reality we only need to calculate the lower triangular part of this matrix.

Summarizing the considerations of Sections 2 and 3, let us write the following procedure to calculate the elements of the inverse matrix $A^{-1}=\left[x_{i j}\right]_{n \times n}$ for nonsingular matrix $A$ given in (1).

## Procedure Inv 3d Hermitian

1. Input elements $a_{1}, a_{2}, \ldots, a_{n}$ and $b_{1}, b_{2}, \ldots, b_{n-1}$ of the matrix $A$ (see (1)).
2. Calculate the quantities $f_{i}, g_{i}, p$ and $q$ (see (5)):

$$
f_{i}=\frac{a_{i}}{\overline{b_{i-1}}}, g_{i}=\frac{b_{i}}{\overline{b_{i-1}}}, i=2,3, \ldots, n-1 ; p=\frac{a_{1}}{b_{1}}, q=\frac{a_{n}}{\overline{b_{n-1}}} .
$$

3. Calculate recursively the quantities $\mu_{i}$ (see (7)):

$$
\begin{aligned}
& \mu_{n}=1, \mu_{n-1}=-q \\
& \mu_{i}=-f_{i+1} \mu_{i+1}-g_{i+1} \mu_{i+2}, i=n-2, n-3, \ldots, 1
\end{aligned}
$$

4. Calculate recursively the quantities $\nu_{i}$ (see (14)):

$$
\begin{aligned}
& \nu_{1}=1, \nu_{2}=-p, \\
& \nu_{i}=-\frac{1}{g_{i-1}}\left(\nu_{i-2}+f_{i-1} \nu_{i-1}\right), i=3,4, \ldots, n .
\end{aligned}
$$

5. Calculate the quantity $t$ (see (10) and Remark 1 ):

$$
t=\left(a_{1} \mu_{1}+b_{1} \mu_{2}\right)^{-1}
$$

6. Calculate the lower triangular part of the matrix $A^{-1}$ (see (37)):

$$
x_{i j}=t \mu_{i} \overline{\nu_{j}}, i=j, j+1, \ldots, n ; \quad j=1,2, \ldots, n .
$$

7. Set the upper triangular part of the matrix $A^{-1}$ (see (37)):

$$
x_{i j}=\overline{x_{j i}}, i=1,2, \ldots, j-1 ; \quad j=2,3, \ldots, n .
$$

8. Output the matrix $A^{-1}=\left[x_{i j}\right]_{n \times n}$.

## End procedure

The procedure Inv 3d Hermitian can be useful for the following purposes. Firstly, it can be used as a basis of numerical algorithms for inverting nonsingular tridiagonal Hermitian matrices. In this case, it is easy to make sure that computing the lower triangular part of the matrix $A^{-1}$ requires $0.5 n^{2}+O(n)$ arithmetical operations with complex numbers. Secondly, for matrices of special types, the procedure can be used for deriving closed form expressions for the elements of inverse matrices. The next section is devoted to this issue.

## 4. Toeplitz Tridiagonal Hermitian Matrices

Let us consider a matrix

$$
A=\left[\begin{array}{ccccc}
a & b & & &  \tag{38}\\
\bar{b} & a & b & & 0 \\
& \ddots & \ddots & \ddots & \\
0 & & \bar{b} & a & b \\
& & & \bar{b} & a
\end{array}\right]
$$

of order $n$, where $a$ is a real number and $b \neq 0$. Additionally, we assume that

$$
\begin{equation*}
|a| \geq 2|b| \tag{39}
\end{equation*}
$$

Condition (39) ensures the nonsingularity of the matrix (38) (see [11], for instance).
For the matrix we are considering, the quantities calculated in Item 2 of the procedure Inv 3d Hermitian are as follows:

$$
f_{i}=\frac{a}{\bar{b}}, g_{i}=\frac{b}{\bar{b}}, i=2,3, \ldots, n-1 ; p=\frac{a}{b}, q=\frac{a}{\bar{b}} .
$$

Further, in Item 3 of the procedure, the quantities $\mu_{i}$ are calculated. In our case, we have second-order recurrent relations

$$
\bar{b} \mu_{i}+a \mu_{i+1}+b \mu_{i+2}=0, i=n-2, n-3, \ldots, 1,
$$

where $\mu_{n}=1, \mu_{n-1}=-a / \bar{b}$. The solution of this problem is well known (see [2, 6], for instance). As a result of calculations, we get that

$$
\begin{equation*}
\mu_{i}=(-1)^{n-i} \frac{\bar{b}}{r}\left[\left(\frac{a+r}{2 \bar{b}}\right)^{n+1-i}-\left(\frac{a-r}{2 \bar{b}}\right)^{n+1-i}\right], i=1,2, \ldots, n \quad \text { if }|a|>2|b| \tag{40}
\end{equation*}
$$

and

$$
\begin{equation*}
\mu_{i}=(-1)^{n-i}(n+1-i)\left(\frac{a}{2 b}\right)^{i-n}, i=1,2, \ldots, n \quad \text { if }|a|=2|b|, \tag{41}
\end{equation*}
$$

where

$$
r \equiv \sqrt{a^{2}-4|b|^{2}}
$$

In a similar way, we find expressions for the quantities $\nu_{i}$ determined in Item 4 of the procedure. These quantities satisfy the following second-order recurrent relations:

$$
\bar{b} \nu_{i-2}+a \nu_{i-1}+b \nu_{i}=0, i=3,4, \ldots, n,
$$

where $\nu_{1}=1, \nu_{2}=-a / b$. Making calculations, we find that

$$
\begin{equation*}
\nu_{i}=(-1)^{i-1} \frac{b}{r}\left[\left(\frac{a+r}{2 b}\right)^{i}-\left(\frac{a-r}{2 b}\right)^{i}\right], i=1,2, \ldots, n \quad \text { if }|a|>2|b| \tag{42}
\end{equation*}
$$

and

$$
\begin{equation*}
\nu_{i}=(-1)^{i-1} i\left(\frac{a}{2 b}\right)^{i-1}, i=1,2, \ldots, n \quad \text { if }|a|=2|b| . \tag{43}
\end{equation*}
$$

In Item 5 of the procedure, the quantity $t$ is calculated. Using the expressions (40) and (41), we get

$$
\begin{equation*}
t=(-1)^{n-1} \frac{r}{\bar{b}^{2}}\left[\left(\frac{a+r}{2 \bar{b}}\right)^{n+1}-\left(\frac{a-r}{2 \bar{b}}\right)^{n+1}\right]^{-1} \quad \text { if }|a|>2|b| \tag{44}
\end{equation*}
$$

and

$$
\begin{equation*}
t=\frac{(-1)^{n-1}}{n+1} \frac{2}{a}\left(\frac{a}{2 b}\right)^{n-1} \quad \text { if }|a|=2|b| . \tag{45}
\end{equation*}
$$

Finally, in Items 6 and 7 of the procedure, the elements $x_{i j}$ of the inverse matrix $A^{-1}$ are calculated. If $|a|>2|b|$, then we use the formulas (40), (42) and (44). For the values $j=1,2, \ldots, n$, we obtain that

$$
\begin{equation*}
x_{i j}=\frac{(-1)^{j-i}}{r} \frac{\left[\left(\frac{a+r}{2 b}\right)^{i}-\left(\frac{a-r}{2 b}\right)^{i}\right]\left[\left(\frac{a+r}{2 b}\right)^{n+1-j}-\left(\frac{a-r}{2 b}\right)^{n+1-j}\right]}{\left[\left(\frac{a+r}{2 b}\right)^{n+1}-\left(\frac{a-r}{2 b}\right)^{n+1}\right]} \tag{46}
\end{equation*}
$$

if $i=1,2, \ldots, j-1$ and

$$
\begin{equation*}
x_{i j}=\frac{(-1)^{i-j}}{r} \frac{\left[\left(\frac{a+r}{2 \bar{b}}\right)^{n+1-i}-\left(\frac{a-r}{2 \bar{b}}\right)^{n+1-i}\right]\left[\left(\frac{a+r}{2 \bar{b}}\right)^{j}-\left(\frac{a-r}{2 \bar{b}}\right)^{j}\right]}{\left[\left(\frac{a+r}{2 \bar{b}}\right)^{n+1}-\left(\frac{a-r}{2 \bar{b}}\right)^{n+1}\right]} \tag{47}
\end{equation*}
$$

if $i=j, j+1, \ldots, n$. As an example, consider the matrix

$$
A=\left[\begin{array}{ccccc}
5 & 2 \mathrm{i} & & & \\
-2 \mathrm{i} & 5 & 2 \mathrm{i} & & 0 \\
& \ddots & \ddots & \ddots & \\
0 & & -2 \mathrm{i} & 5 & 2 \mathrm{i} \\
& & & -2 \mathrm{i} & 5
\end{array}\right]
$$

According to the expressions (46) and (47) we find that

$$
x_{i j}=\left\{\begin{array}{l}
\frac{\left(2^{i}-2^{-i}\right)\left(2^{n+1-j}-2^{-n-1+j}\right)}{3\left(2^{n+1}-2^{-n-1}\right)} \mathrm{i}^{i-j}, i=1,2, \ldots, j-1, \\
\frac{\left(2^{n+1-i}-2^{-n-1+i}\right)\left(2^{j}-2^{-j}\right)}{3\left(2^{n+1}-2^{-n-1}\right)} \mathrm{i}^{i-j}, i=j, j+1, \ldots, n,
\end{array}\right.
$$

where the symbol i stands for the imaginary unit.
Now consider the case $|a|=2|b|$. For the values $j=1,2, \ldots, n$, using the formulas (41), (43) and (45), we find that

$$
x_{i j}=\left\{\begin{array}{l}
(-1)^{j-i} \frac{(n+1-j) i}{n+1} \frac{2}{a}\left(\frac{a}{2 b}\right)^{i-1}\left(\frac{a}{2 \bar{b}}\right)^{j-1}, i=1,2, \ldots, j-1,  \tag{48}\\
(-1)^{i-j} \frac{(n+1-i) j}{n+1} \frac{2}{a}\left(\frac{a}{2 b}\right)^{i-1}\left(\frac{a}{2 \bar{b}}\right)^{j-1}, i=j, j+1, \ldots, n
\end{array}\right.
$$

For the matrix

$$
A=\left[\begin{array}{ccccc}
2 & \mathrm{i} & & & \\
-\mathrm{i} & 2 & \mathrm{i} & & 0 \\
& \ddots & \ddots & \ddots & \\
0 & & -\mathrm{i} & 2 & \mathrm{i} \\
& & & -\mathrm{i} & 2
\end{array}\right]
$$

the expressions (48) take the following form:

$$
x_{i j}=\left\{\begin{array}{l}
(-1)^{j} \frac{(n-j+1) i}{n+1} \mathrm{i}^{i+j}, i=1,2, \ldots, j-1, \\
(-1)^{j} \frac{(n-i+1) j}{n+1} \mathrm{i}^{i+j}, i=j, j+1, \ldots, n,
\end{array} \quad j=1,2, \ldots, n .\right.
$$

## 5. Conclusion

In this paper, we have constructed the computational procedure Inv 3d Hermitian for inversion of tridiagonal Hermitian matrices. This procedure can be used as a numerical algorithm with an optimal number of arithmetic operations (see the comment on the procedure at the end of Section 3). In certain cases, the procedure can also be used to derive closed-form expressions for the elements of inverse matrices. In this regard, Toeplitz tridiagonal Hermitian matrices in Section 4 were considered.

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<br><br>e-mail: yuri.hakopian@ysu.am, avetiq.manukyan1@ysumail.am

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# Аналитическое обращение трехдиагональных изображени 

Юрий Р. Акопян и Аветик А. Манукян<br>Ереванский государственный университет, Ереван, Армения<br>e-mail: yuri.hakopian@ysu.am, avetiq.manukyan1@ysumail.am


#### Abstract

Аннотация В статье дается алгоритм обращения трехдиагональных эрмитовых матриц, численная реализация которого осуществляется за оптимальное число арифметических операций. Вычислительная процедура представляет собой


последовательность рекуррентных соотношений, приводящих к вычислению элементов обратной матрицы. Для матриц специального типа и, в частности, для тёплицевых трехдиагональных эрмитовых матриц, полученные соотношения приводят к явным формулам для элементов обратной матрицы.

Ключевые слова: обратная матрица, трехдиагональная матрица, эрмитова матрица, тёплицева матрица.

# On an Extension of the Ghouila-Houri Theorem 

Samvel Kh. Darbinyan<br>Institute for Informatics and Automation Problems of NAS RA<br>e-mail: samdarbin@iiap.sci.am


#### Abstract

Let $D$ be a 2 -strong digraph of order $n \geq 8$ such that for every vertex $x \in \mathcal{V}(\mathcal{D}) \backslash\{z\}$, $d(x) \geq n$ and $d(z) \geq n-4$, where $z$ is a vertex in $\mathcal{V}(\mathcal{D})$. We prove that:

If $D$ contains a cycle passing through $z$ of length equal to $n-2$, then $D$ is Hamiltonian.

We also give a new sufficient condition for a digraph to be Hamiltonian-connected. Keywords: Digraphs, Hamiltonian cycles, Hamiltonian-connected, 2-strong. Article info: Received 21 April 2022; received in revised form 16 September 2022; accepted 15 November 2022. Acknowledgement: We thank the referees for their valuable comments and suggestions that improved the presentation considerably.


## 1. Introduction

In this paper, we consider finite digraphs (directed graphs) without loops and multiple arcs. The order of a digraph $D$ is the number of its vertices. We shall assume that the reader is familiar with the standard terminology on digraphs. Terminology and notations not described below follow [1]. Every cycle and path is assumed simple and directed. A cycle (path) in a digraph $D$ is called Hamiltonian (Hamiltonian path) if it includes every vertex of $D$. A digraph $D$ is Hamiltonian if it contains a Hamiltonian cycle, and it is Hamiltonianconnected if for any pair of ordered vertices $x$ and $y$ there exists a Hamiltonian path from $x$ to $y$.

There are numerous sufficient conditions for the existence of a Hamiltonian cycle in a digraph (see, [1]-[3]). Let us recall the following sufficient conditions for a digraph to be Hamiltonian.

Theorem 1: (Ghouila-Houri [4]). Let $D$ be a strong digraph of order $n \geq 2$. If for every vertex $x \in \mathcal{V}(\mathcal{D}), d(x) \geq n$, then $D$ is Hamiltonian.

Theorem 2: (Meyniel [5]). Let $D$ be a strong digraph of order $n \geq 2$. If $d(x)+d(y) \geq 2 n-1$ for all pairs of non-adjacent vertices $x$ and $y$ in $D$, then $D$ is Hamiltonian.

Nash-Williams [6] raised the problem of describing all the extreme digraphs in Theorem 1, that is, all digraphs with minimum degree at least $|D|-1$, that do not have a Hamiltonian
cycle. As a solution to this problem, Thomassen [7] proved a structural theorem on the extreme digraphs. An analogous problem for Theorem 2 was considered by the author [8]. In [8], we generalize Thomassen's structural theorem (Theorem 1, in [7]), characterizing the nonHamiltonian strong digraphs of order $n$ with the degree condition that $d(x)+d(y) \geq 2 n-2$ for every pair of non-adjacent distinct vertices $x, y$. Moreover, in [8], it was also proved that if $m$ is the length of a longest cycle in $D$, then $D$ contains cycles of all lengths $k=2,3, \ldots, m$. The following conjecture was suggested by Thomassen.

Conjecture 1: (Thomassen [9], see Conjecure 1.6.7 in [2]). Every 3-strong digraph of order $n$ and with minimum degree at least $n+1$ is Hamiltonian-connected.

In [10], we disprove this conjecture, by proving the following three theorems.
Theorem 3: Every $k$-strong ( $k \geq 1$ ) digraph of order $n$, which has $n-1$ vertices of degrees at least $n$, is Hamiltonian if and only if any $(k+1)$-strong digraph of order $n+1$ with minimum degree at least $n+2$ is Hamiltonian-connected.

Theorem 4: For every $n \geq 8$, there is a non-Hamiltonian 2-strong digraph $D$ of order $n$ with minimum degree equal to 4 such that $D$ has $n-1$ vertices of degrees at least $n$.

Theorem 5: For every $n \geq 9$, there exists a 3-strong digraph $D$ of order $n$ with minimum degree at least $n+1$ such that $D$ contains two distinct vertices $u, v$ for which $u \leftrightarrow v, d_{D}^{+}(u)+$ $d_{D}^{-}(v)=6$ and there is no $(u, v)$-Hamiltonian path.

In view of Theorems 4,5 and Conjecture 1, it is natural to pose the following problem.
Problem: Let $D$ be a 2-strong digraph of order $n \geq 9$. Suppose that $n-1$ vertices of $D$ have degrees at least $n$ and a vertex $x$ has degree is at least $n-m$, where $1 \leq m \leq n-5$. Find the maximum value of $m$, for which $D$ is Hamiltonian.

Goldberg, Levitskaya and Satanovskiy [11] relaxed the conditions of the Ghouila-Houri theorem. They proved the following theorem.

Theorem 6: (Goldberg et al. [11]). Let $D$ be a strong digraph of order $n \geq 2$. If for every vertex $x \in \mathcal{V}(D) \backslash\{z\}, d(x) \geq n$ and $d(z) \geq n-1$, then $D$ is Hamiltonian.

Note that Theorem 6 is an immediate consequence of Theorem 2. In [11], the authors for any $n \geq 5$ presented two examples of non-Hamiltonian strong digraphs of order $n$ such that:
(i) In the first example, $n-2$ vertices have degrees equal to $n+1$ and the other two vertices have degrees equal to $n-1$.
(ii) In the second example, $n-1$ vertices have degrees at least $n$ and the remaining vertex has degree equal to $n-2$.

In [12], it was reported that the following theorem holds.
Theorem 7: (Darbinyan [12]). Let $D$ be a 2-strong digraph of order $n \geq 9$ with minimum degree at least $n-4$. If $n-1$ vertices of $D$ have degrees at least $n$, then $D$ is Hamiltonian.

In this article, we present the first part of the proof of Theorem 7, which we formulate as Theorem 9. The proof of the last theorem has never been published. It is worth mentioning that the proof presented here differs from the previous handwritten proof and is significantly shorter and more general than the previous one. The second part of the proof (i.e., the complete proof) of Theorem 7 we will present in the forthcoming paper, where we also
present two examples of digraphs, which show that the bounds $n \geq 9$ and $n-4$ in Theorem 7 are sharp in a sense.

## 2. Further Terminology and Notation

For the sake of clarity we repeat the most impotent definition. The vertex set and the arc set of a digraph $D$ are denoted by $\mathcal{V}(\mathcal{D})$ and $\mathcal{A}(\mathcal{D})$, respectively. The order of a digraph $D$ is the number of its vertices. The converse digraph of $D$ is the digraph obtained from $D$ by reversing the direction of all arcs. The arc of a digraph $D$ directed from $x$ to $y$ is denoted by $x y$ or $x \rightarrow y$ (we also say that $x$ dominates $y$ or $y$ is an out-neighbour of $x$ and $x$ is an in-neighbour of $y$ ), and $x \leftrightarrow y$ denotes that $x \rightarrow y$ and $y \rightarrow x(x \leftrightarrow y$ is called 2-cycle). If $x \rightarrow y$ and $y \rightarrow z$, we write $x \rightarrow y \rightarrow z$. If $A$ and $B$ are two disjoint subsets of $\mathcal{V}(\mathcal{D})$ such that every vertex of $A$ dominates every vertex of $B$, then we say that $A$ dominates $B$, denoted by $A \rightarrow B$. We define $\mathcal{A}(A \rightarrow B)=\{x y \in \mathcal{A}(D) \mid x \in A, y \in B\}$ and $\mathcal{A}(\mathcal{A}, \mathcal{B})=\mathcal{A}(\mathcal{A} \rightarrow \mathcal{B}) \cup \mathcal{A}(\mathcal{B} \rightarrow \mathcal{A})$. If $x \in \mathcal{V}(\mathcal{D})$ and $A=\{x\}$ we sometimes write $x$ instead of $\{x\}$. Let $N_{D}^{+}(x), N_{D}^{-}(x)$ denote the set of out-neighbors, respectively the set of in-neighbors of a vertex $x$ in a digraph $D$. If $A \subseteq \mathcal{V}(\mathcal{D})$, then $N_{D}^{+}(x, A)=A \cap N_{D}^{+}(x)$ and $N_{D}^{-}(x, A)=A \cap N_{D}^{-}(x)$. The outdegree of $x$ is $d_{D}^{+}(x)=\left|N_{D}^{+}(x)\right|$ and $d_{D}^{-}(x)=\left|N_{D}^{-}(x)\right|$ is the in-degree of $x$. Similarly, $d_{D}^{+}(x, A)=\left|N_{D}^{+}(x, A)\right|$ and $d_{D}^{-}(x, A)=\left|N_{D}^{-}(x, A)\right|$. The degree of the vertex $x$ in $D$ is defined as $d_{D}(x)=d_{D}^{+}(x)+d_{D}^{-}(x)$ (similarly, $d_{D}(x, A)=d_{D}^{+}(x, A)+d_{D}^{-}(x, A)$ ). We omit the subscript if the digraph is clear from the context. The subdigraph of $D$ induced by a subset $A$ of $\mathcal{V}(\mathcal{D})$ is denoted by $D$. In particular, $D-A=D\langle\mathcal{V}(\mathcal{D}) \backslash \mathcal{A}\rangle$. For integers $a$ and $b$, $a \leq b$, by $[a, b]$ we denote the set $\left\{x_{a}, x_{a+1}, \ldots, x_{b}\right\}$. If $j<i$, then $\left\{x_{i}, \ldots, x_{j}\right\}=\emptyset$.

The path (respectively, the cycle) consisting of the distinct vertices $x_{1}, x_{2}, \ldots, x_{m}(m \geq 2)$ and the arcs $x_{i} x_{i+1}, i \in[1, m-1]$ (respectively, $x_{i} x_{i+1}, i \in[1, m-1]$, and $x_{m} x_{1}$ ), is denoted by $x_{1} x_{2} \cdots x_{m}$ (respectively, $x_{1} x_{2} \cdots x_{m} x_{1}$ ). The length of a cycle or a path is the number of its arcs. Let $D$ be a digraph and $z \in \mathcal{V}(\mathcal{D})$. By $C_{m}(z)$ (respectively, $C(z)$ ) we denote a cycle in $D$ of length $m$ (respectively, any cycle in $D$ ), which contains the vertex $z$. We say that $P=x_{1} x_{2} \cdots x_{m}$ is a path from $x_{1}$ to $x_{m}$ or is an $\left(x_{1}, x_{m}\right)$-path. A digraph $D$ is strong (strongly connected) if, for every pair $x, y$ of distinct vertices in $D$, there exists an $(x, y)$-path and a ( $y, x$ )-path. A digraph $D$ is $k$-strong ( $k$-strongly connected) if, $|\mathcal{V}(\mathcal{D})| \geq \|+\infty$ and for any set $A$ of at most $k-1$ vertices $D-A$ is strong. Two distinct vertices $x$ and $y$ are adjacent if $x y \in$ or $y x \in \mathcal{A}(\mathcal{D})$ (or both). The converse digraph of $D$ is the digraph obtained from $D$ by replacing the direction of all arcs. We will use the principle of digraph duality: Let $D$ be a digraph, then $D$ contains a subdigraps $H$ if and only if the converse digraph of $D$ contain the converse of subdigraph $H$.

## 3. Preliminaries

In our proofs, we will use the following well-known simple lemma.
Lemma 1: (Häggkvist and Thomassen [13]). Let $D$ be a digraph of order $n \geq 3$ containing a cycle $C_{m}$ of length $m, m \in[2, n-1]$. Let $x$ be a vertex not contained in this cycle. If $d\left(x, \mathcal{V}\left(C_{m}\right)\right) \geq m+1$, then for every $k \in[2, m+1], D$ contains a cycle $C_{k}$ including $x$.

The next lemma is a slight modification of a lemma by Bondy and Thomassen [14], it is very useful and will be used extensively throughout this paper.

Lemma 2:. Let $D$ be a digraph of order $n \geq 3$ containing a path $P:=x_{1} x_{2} \ldots x_{m}, m \in$ $[2, n-1]$. Let $x$ be a vertex not contained in this path. If one of the following condition holds:
(i) $d(x, \mathcal{V}(P)) \geq m+2$,
(ii) $d(x, \mathcal{V}(P)) \geq m+1$ and $x x_{1} \notin \mathcal{A}(D)$ or $x_{m} x \notin \mathcal{A}(\mathcal{D})$,
(iii) $d(x, \mathcal{V}(P)) \geq m$ and $x x_{1} \notin \mathcal{A}(\mathcal{D})$ and $x_{m} x \notin \mathcal{A}(\mathcal{D})$,
then there is an $i \in[1, m-1]$ such that $x_{i} \rightarrow x \rightarrow x_{i+1}$, i.e., $D$ contains a path $x_{1} x_{2} \ldots x_{i} x x_{i+1} \ldots x_{m}$ of length $m$ (we say that $x$ can be inserted into $P$ ).

Using Lemma 2, we can prove the following lemma.
Lemma 3: Let $P:=x_{1} x_{2} \ldots x_{m}, m \in[3, n-1]$, be a longest $\left(x_{1}, x_{m}\right)$-path in a digraph $D$ of order $n$. Suppose that $y \in \mathcal{V}(D) \backslash \mathcal{V}(P)$ and there is no $i \in[1, m-2]$ such that $x_{i} \rightarrow y \rightarrow x_{i+2}$. Then the following holds:
(i) If $y x_{1} \notin \mathcal{A}(\mathcal{D}), x_{1} y \in \mathcal{A}(\mathcal{D})$ and $d(y, \mathcal{V}(P)) \geq m$, then $d(y, \mathcal{V}(P))=m$ and $\left\{x_{1}, x_{2}, \ldots, x_{m}\right\} \rightarrow y$;
(ii) If $x_{m} y \notin \mathcal{A}(\mathcal{D}), y x_{m} \in \mathcal{A}(\mathcal{D})$ and $d(y, \mathcal{V}(P)) \geq m$, then $d(y, \mathcal{V}(P))=m$ and $y \rightarrow\left\{x_{1}, x_{2}, \ldots, x_{m}\right\} ;$
(iii) If $d(y, \mathcal{V}(P)) \geq m+1$, then $d(y, \mathcal{V}(P))=m+1$ and there exists an integer $q \in[1, m]$ such that $\left\{x_{q}, x_{q+1}, \ldots, x_{m}\right\} \rightarrow y \rightarrow\left\{x_{1}, x_{2}, \ldots, x_{q}\right\}$.

Proof. To prove the lemma, it suffices to show that every vertex $x_{i} \in \mathcal{V}(\mathcal{P})$ is adjacent to $y$. Assume that this is not the case. (i) Let $y$ and $x_{t}$ be not adjacent. Then $t \geq 2$ since $x_{1} \rightarrow y$. Since $P$ is a longest $\left(x_{1}, x_{m}\right)$-path, we have that $y$ cannot be inserted into $P$. Using Lemma 2(ii) and the assumption that $y x_{1} \notin \mathcal{A}(\mathcal{D})$, we obtain $x_{m} y \in \mathcal{A}(\mathcal{D}), 2 \leq t \leq m-1$ and

$$
m \leq d(y, \mathcal{V}(P))=d\left(y,\left\{x_{1}, \ldots, x_{t-1}\right\}\right)+d\left(y,\left\{x_{t+1}, \ldots, x_{m}\right\}\right) \leq t-1+(m-t+1)=m
$$

This means that $d\left(y,\left\{x_{1}, \ldots, x_{t-1}\right\}\right)=t-1$ and $d\left(y,\left\{x_{t+1}, \ldots, x_{m}\right\}\right)=m-t+1$. Again using Lemma 2, we obtain that $x_{t-1} \rightarrow y \rightarrow x_{t+1}$, which contradicts the supposition of Lemma 3. This contradiction shows that every vertex $x_{i}$ is adjacent to $y$.

In a similar way, one can show that if (ii) or (iii) holds, then every vertex of $P$ also is adjacent to $y$. Lemma 3 is proved.

In [10], the author proved the following theorem.
Theorem 8: (Darbinyan [12]). Let $D$ be a strong digraph of order $n \geq 3$. Suppouse that $d(x)+d(y) \geq 2 n-1$ for all pairs of non-adjacent vertices $x, y \in \mathcal{V}(D) \backslash\{z\}$, where $z$ is some vertex in $\mathcal{V}(\mathcal{D})$. Then $D$ is Hamiltonian or contains a cycle of length $n-1$.

Using Theorem 8 and Lemmas 1 and 2, it is not difficult to show that the following corollaries are true.

Corollary 1: Let $D$ be a strong digraph of order $n \geq 3$ satisfying the condition of Theorem 8. Then $D$ has a cycle that contains all the vertices of $D$ maybe except $z$.

Corollary 2: Let $D$ be a strong digraph of order $n \geq 3$. Suppose that $n-1$ vertices of $D$ have degrees at least $n$. Then $D$ is Hamiltonian or contains a cycle of length $n-1$ (in fact, $D$ has a cycle that contains all the vertices of degrees at least $n$ ).

In this section, we also will prove the following lemma. We will use this lemma in the second part of the proof of Theorem 7.

Lemma 4: Let $D$ be a digraph of order $n \geq 4$ such that for any vertex $x \in \mathcal{V}(D) \backslash\{z\}, d(x) \geq$ $n$ and $d(z) \leq n-2$, where $z$ is some vertex in $\mathcal{V}(\mathcal{D})$. Suppose that $C_{m}(z)=x_{1} x_{2} \ldots x_{m} x_{1}$ with $m \leq n-2$ is a longest cycle through $z$. If $D\left\langle V(D) \backslash V\left(C_{m}(z)\right)\right\rangle$ is strong and $D$ contains a $C_{m}(z)$-bypass $P=x_{i} y_{1} y_{2} \ldots y_{l} x_{j}$ such that $\left|\mathcal{V}\left(C_{m}(z)\left[x_{i+1}, x_{j-1}\right]\right)\right|$ is smallest possible over all $C_{m}(z)$-bypasses, then $z \in \mathcal{V}\left(C_{m}(z)\left[x_{i+1}, x_{j-1}\right]\right)$.

Proof. Without loss of generality, we assume that $x_{j}=x_{1}, x_{i}=x_{m-k}, k \geq 1$, $\mathcal{A}\left(\left\{y_{1}, \ldots, y_{l}\right\}, \mathcal{V}\left(C_{m}(z)\left[x_{m-k+1}, x_{m}\right]\right)\right)=\emptyset$ and $k$ is minimum possible with this property over all $C_{m}(z)$-bypasses. Extending the path $C_{m}(z)\left[x_{1}, x_{m-k}\right]$ with the vertices of $\mathcal{V}\left(C_{m}(z)\left[x_{m-k+1}, x_{m}\right]\right)$ as much as possible, we obtain an $\left(x_{1}, x_{m-k}\right)$-path, say $R$. Since $C_{m}(z)$ is a longest cycle through $z$, some vertices $u_{1}, u_{2}, \ldots, u_{d} \in \mathcal{V}\left(C_{m}(z)\left[x_{m-k+1}, x_{m}\right]\right)$, $1 \leq d \leq k$, are not on the obtained extended path $R$. Using Lemma 2, we obtain that $d\left(y_{i}, \mathcal{V} V\left(C_{m}(z)\right)\right) \leq m-k+1$ and $d\left(u_{i}, \mathcal{V}\left(C_{m}(z)\right)\right) \leq m+d-1$. Put $B:=\mathcal{V}(D) \backslash\left(\mathcal{V}\left(C_{m}(z)\right) \cup \mathcal{V}(\mathcal{P})\right)$. Note that $|B|=n-m-l$. Let $v$ be an arbitrary vertex in $B$. From the minimality of $k$, we have that $D$ contains no paths of the types $u_{i} \rightarrow v \rightarrow y_{j}$ and $y_{j} \rightarrow v \rightarrow u_{i}$, which in turn implies that $d^{+}\left(u_{i}, B\right)+d^{-}\left(y_{j}, B\right) \leq|B|$ and $d^{-}\left(u_{i}, B\right)+d^{+}\left(y_{j}, B\right) \leq|B|$. Therefore, $d\left(u_{i}, B\right)+d\left(y_{j}, B\right) \leq 2|B|=2(n-m-l)$. Thus, we have

$$
\begin{aligned}
d\left(u_{i}\right) & +d\left(y_{j}\right)=d\left(u_{i}, \mathcal{V}\left(C_{m}(z)\right)\right)+d\left(y_{j}, \mathcal{V}\left(C_{m}(z)\right)\right)+d\left(u_{i}, B\right)+d\left(y_{j}, B\right)+d\left(y_{j},\left\{y_{1}, \ldots, y_{l}\right\}\right) \\
& \leq m+d-1+m-k+1+2 n-2 m-2 l+2 l-2=2 n-2-(k-d) \leq 2 n-2
\end{aligned}
$$

This is possible if $u_{i}=z$. Therefore, $d=1$ and $z \in \mathcal{V}\left(C_{m}(z)\left[x_{m-k+1}, x_{m}\right]\right)$. Lemma 4 is proved.

## 4. The Main Result

In this section, we prove the following theorem.
Theorem 9: Let $D$ be a 2-strong digraph of order $n \geq 8$. Suppose that for every $x \in$ $\mathcal{V}(D) \backslash\{z\}, d(x) \geq n$ and $d(z) \geq n-4$, where $z$ is a vertex in $\mathcal{V}(\mathcal{D})$. If $D$ contains a cycle of length $n-2$ passing through $z$ (i.e., a cycle $C_{n-2}(z)$ ), then $D$ is Hamiltonian.

Before we prove our main result, we will prove the following lemma.
Lemma 5: Let $D$ be a non-Hamiltonian 2-strong digraph of order $n$ such that for any vertex $x \in \mathcal{V}(D) \backslash\{z\}, d(x) \geq n$ and $d(z) \leq n-2$, where $z$ is an arbitrary fixed vertex in $\mathcal{V}(\mathcal{D})$. Suppose that $C_{m+1}(z)=x_{1} x_{2} \ldots x_{m} z x_{1}$ with $m \in[2, n-3]$ is a longest cycle in $D$, $d(z, Y)=0$ and $D\langle Y\rangle$ is a strong digraph, where $Y:=\mathcal{V}(D) \backslash \mathcal{V}\left(C_{m+1}(z)\right)$. Let $y_{1}, y_{2}$ be two distinct vertices in $Y$. If for each $y_{i} \in\left\{y_{1}, y_{2}\right\}, d\left(y_{i},\left\{x_{1}, x_{2}, \ldots, x_{m}\right\}\right)=m+1$, then $n \geq 6$ and $d(z) \leq m-2$.

Proof. By contradiction, suppose that $d(z) \geq m-1$. We denote by $P$ the path $x_{1} x_{2} \ldots x_{m}$. Note that $|Y|=n-m-1$. Since the path $P$ cannot be extended with any vertex $y \in Y$, by Lemma $2, d(y, \mathcal{V}(P)) \leq m+1$ and

$$
\begin{equation*}
n \leq d(y)=d(y, \mathcal{V}(P))+d(y, Y) \leq m+1+d(y, Y), d(y, Y) \geq n-m-1=|Y| . \tag{1}
\end{equation*}
$$

Since $D$ is 2-strong and $C_{m+1}(z)$ is a longest cycle, using Lemma 2 and $d\left(y_{i}, \mathcal{V}(P)\right)=m+1$ it is not difficult to show that there is an integer $l \in[2, m-1]$ such that

$$
\begin{equation*}
\left\{x_{l}, x_{l+1}, \ldots, x_{m}\right\} \rightarrow\left\{y_{1}, y_{2}\right\} \rightarrow\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} . \tag{2}
\end{equation*}
$$

Since $d(y, Y) \geq n-m-1=|Y|($ by (1)), and $D\langle Y\rangle$ is strong, by the Ghouila-Houri theorem, $D\langle Y\rangle$ is Hamiltonian. Put $E:=\left\{x_{1}, x_{2}, \ldots, x_{l-1}\right\}$ and $F:=\left\{x_{l+1}, x_{l+2}, \ldots, x_{m}\right\}$. Since $C_{m+1}(z)$ is a longest cycle and $D\langle Y\rangle$ is strong, from (2) it follows that

$$
\begin{equation*}
\mathcal{A}(\mathcal{E} \rightarrow \mathcal{Y})=\mathcal{A}(\mathcal{Y} \rightarrow \mathcal{F})=\emptyset \tag{3}
\end{equation*}
$$

Note that from $|Y| \geq 2,|E| \geq 1$ and $|F| \geq 1$ it follows that $n \geq 6$. We need to prove the following Claims 1-2 bellow.

## Claim 1.

(i) If $d^{-}(z, E) \geq 1$, then $d^{+}(z, F)=0$.
(ii) $\mathcal{A}(\mathcal{E} \rightarrow \mathcal{F}) \neq \emptyset$.

Proof. (i) By contradiction, suppose that $x_{i} \in E, x_{j} \in F$ and $x_{i} \rightarrow z \rightarrow x_{j}$. Then by (2), $y_{1} \rightarrow x_{i+1}$ and $x_{j-1} \rightarrow y_{2}$. Hence, $C_{m+3}(z)=x_{1} x_{2} \ldots x_{i} z x_{j} \ldots x_{m} y_{1} x_{i+1} \ldots x_{j-1} y_{2} x_{1}$, a contradiction.
(ii) Suppose, on the contrary, that $\mathcal{A}(\mathcal{E} \rightarrow \mathcal{F})=\emptyset$. Then using Claim 1(i) and (3), we obtain: if $d^{-}(z, E) \geq 1$, then $d^{+}(z, F)=0$ and $\mathcal{A}(E \cup Y \cup\{z\} \rightarrow F)=\emptyset$, if $d^{-}(z, E)=0$, then $\mathcal{A}(E \cup Y \rightarrow F \cup\{z\})=\emptyset$. Therefore, $D-x_{l}$ is not strong, which contradicts that $D$ is 2 -strong.

From now on, we assume that $x_{a} x_{b} \in \mathcal{A}(\mathcal{E} \rightarrow \mathcal{F})$. Note that $1 \leq a \leq l-1$ and $l+1 \leq b \leq m$. We may assume that $b$ is the maximum and $a$ is the minimum with these properties. By (2), we have

$$
\begin{equation*}
x_{b-1} \rightarrow\left\{y_{1}, y_{2}\right\} \rightarrow x_{a+1} . \tag{4}
\end{equation*}
$$

Since $z$ cannot be inserted into $P$, using Lemma 2(ii) and Clam 1(i), we obtain

$$
\begin{equation*}
d\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a}\right\}\right)+d\left(z,\left\{x_{b}, x_{b+1}, \ldots, x_{m}\right\}\right) \leq a+m-b+2 . \tag{5}
\end{equation*}
$$

By $R\left(y_{i}, y_{3-i}\right)$, where $i \in[1,2]$, we denote a longest $\left(y_{i}, y_{3-i}\right)$-path in $D\langle Y\rangle$. From now on, assume that $R\left(y_{i}, y_{3-i}\right)=R\left(y_{1}, y_{2}\right)$.

## Claim 2.

(i) If $i \in[a+1, l-1]$, then $x_{i} z \notin \mathcal{A}(\mathcal{D})$.
(ii) If $j \in[l+1, b-1]$, then $z x_{j} \notin \mathcal{A}(\mathcal{D})$.
(iii) If $i \in[a+1, l]$ and $i-a \leq 2$, then $z x_{i} \notin \mathcal{A}(\mathcal{D})$.
(iv) If $j \in[l, b-1]$ and $b-j \leq 2$, then $x_{j} z \notin \mathcal{A}(\mathcal{D})$.

Proof. Each of claims (i)-(iv) we prove by contradiction.
(i) Assume that $i \in[a+1, l-1]$ and $x_{i} z \in \mathcal{A}(\mathcal{D})$. Then by (2) and (4), we have $C_{m+3}(z)=x_{1} x_{2} \ldots x_{a} x_{b} \ldots x_{m} y_{1} x_{i+1} \ldots x_{b-1} y_{2} x_{a+1} \ldots x_{i} z x_{1}$, a contradiction.
(ii) Assume that $j \in[l+1, b-1]$ and $z x_{j} \in \mathcal{A}(\mathcal{D})$. Then by (2) and (4), we have $C_{m+3}(z)=x_{1} x_{2} \ldots x_{a} x_{b} \ldots x_{m} z x_{j} \ldots x_{b-1} y_{1} x_{a+1} \ldots x_{j-1} y_{2} x_{1}$, a contradiction.
(iii) Assume that $i \in[a+1, l], i-a \leq 2$ and $z x_{i} \in \mathcal{A}(\mathcal{D})$. Then $C(z)=x_{1} x_{2} \ldots x_{a} x_{b} \ldots$ $x_{m} z x_{i} \ldots x_{b-1} R\left(y_{1}, y_{2}\right) x_{1}$ is a cycle of length at least $m+2$, a contradiction.
(iv) Assume that $j \in[l, b-1], b-j \leq 2$ and $x_{j} z \in \mathcal{A}(\mathcal{D})$. Then $C(z)=x_{1} x_{2} \ldots x_{a} x_{b} \ldots$ $x_{m} R\left(y_{1}, y_{2}\right) x_{a+1} \ldots x_{j} z x_{1}$ is a cycle of length at least $m+2$, a contradiction. Claim 2 is proved.

Now we will consider the following cases depending on the values of $a$ and $b$ with respect to $l$.

Case 1. $a \leq l-3$ and $b \geq l+3$.
Then by Claim $2, d\left(z,\left\{x_{a+1}, x_{a+2}, x_{b-2}, x_{b-1}\right\}\right)=0$. Therefore, since $z$ cannot be inserted into $P$, using (5) and Lemma 2, we obtain

$$
\begin{gathered}
m-1 \leq d\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a}, x_{b}, x_{b+1}, \ldots, x_{m}\right\}\right)+d\left(z,\left\{x_{a+3}, \ldots, x_{b-3}\right\}\right) \\
\leq a+m-b+2+b-3-a-2+1=m-2
\end{gathered}
$$

which is a contradiction.
Case 2. $a \leq l-3$ and $b=l+2$.
Then by Claim $2, d\left(z,\left\{x_{a+1}, x_{a+2}, x_{l+1}\right\}\right)=0$ and $x_{l} z \notin \mathcal{A}(\mathcal{D})$. Therefore, since $z$ cannot be inserted into $P$, using (5) and Lemma 2, we obtain

$$
\begin{aligned}
m-1 & \leq d\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a}, x_{b}, x_{b+1}, \ldots, x_{m}\right\}\right)+d\left(z,\left\{x_{a+3}, \ldots, x_{l}\right\}\right) \\
& \leq a+m-b+2+l-a-2=m-(l+2)+l=m-2
\end{aligned}
$$

which is a contradiction.
Case 3. $a \leq l-3$ and $b=l+1$.
Then by Claim 2, $d\left(z,\left\{x_{a+1}, x_{a+2}\right\}\right)=0$ and $x_{l} z \notin \mathcal{A}(\mathcal{D})$. Similar to Case 2, we obtain

$$
\begin{gathered}
m-1 \leq d\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a}, x_{b}, x_{b+1}, \ldots, x_{m}\right\}\right)+d\left(z,\left\{x_{a+3}, \ldots, x_{l}\right\}\right) \\
\leq a+m-b+2+l-a-2=m-b+l=m-(l+1)=m-1
\end{gathered}
$$

This implies that $d\left(z,\left\{x_{a+3}, \ldots, x_{l}\right\}\right)=l-a-2$. Hence, by Claim 2(i) and $x_{l} z \notin \mathcal{A}(\mathcal{D})$, $z \rightarrow\left\{x_{a+3}, \ldots, x_{l}\right\}$. From this and (4), we see that the cycle $Q(z)=x_{1} x_{2} \ldots x_{a} x_{b} \ldots x_{m} z$ $x_{a+3} \ldots x_{l} R\left(y_{1}, y_{2}\right) x_{1}$ has length equal to $m-1+\left|\mathcal{V}\left(R\left(y_{1}, y_{2}\right)\right)\right|$. Since $C_{m+1}(z)$ is a longest cycle and $D\langle Y\rangle$ is Hamiltonian, it follows that $\left|\mathcal{V}\left(R\left(y_{1}, y_{2}\right)\right)\right|=|Y|=2$. Then $m=n-3$, $y_{1} \leftrightarrow y_{2}, x_{a+1} \leftrightarrow x_{a+2}$ and $x_{a+1}\left(x_{a+2}\right)$ is adjacent to each vertex $x_{i} \in\left\{x_{1}, x_{2}, \ldots x_{m}\right\}$, as $d\left(x_{a+1}\right) \geq n\left(d\left(x_{a+2}\right) \geq n\right)$ and $x_{a+1}\left(x_{a+2}\right)$ cannot be inserted into $Q(z)$.

We will distinguish two subcases.
Subcase 3.1. $m \geq l+2$. From the minimality of $a$ and the maximality of $b$, it follows that

$$
\begin{equation*}
\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{a}\right\} \rightarrow\left\{x_{b+1}, x_{b+2}, \ldots, x_{m}\right\}\right)=\emptyset . \tag{6}
\end{equation*}
$$

Assume that $x_{i} \rightarrow x_{j}$ with $i \in[a+1, l]$ and $j \in[l+2, m]$. Using (4) and the fact that $z x_{a+3} \in \mathcal{A}(\mathcal{D})$, it is not difficult to see that if $i \in[a+1, a+2]$, then $C(z)=x_{1} x_{2} \ldots x_{a+1}\left(x_{a+2}\right) x_{j} \ldots x_{m} z x_{a+3} \ldots x_{j-1} y_{1} y_{2} x_{1}$ is a cycle of length at least $m+2$, if $i \in[a+3, l-1]$, then $C_{m+3}(z)=x_{1} x_{2} \ldots x_{i} x_{j} \ldots x_{m} z x_{i+1} \ldots x_{j-1} y_{1} y_{2} x_{1}$, if $i=l$, then $C_{m+3}(z)=x_{1} x_{2} \ldots x_{a} x_{l+1} \ldots x_{j-1} y_{1} y_{2} x_{a+1} \ldots x_{l} x_{j} \ldots x_{m} z x_{1}$. Thus, in all cases, we have a contradiction. We may, therefore, assume that (recall that $b=l+1$ )

$$
\mathcal{A}\left(\left\{x_{a+1}, x_{a+2}, \ldots, x_{l}\right\} \rightarrow\left\{x_{b+1}, x_{b+2}, \ldots, x_{m}\right\}\right)=\emptyset .
$$

Combining this with (6), we obtain

$$
\begin{equation*}
\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \rightarrow\left\{x_{b+1}, x_{b+2}, \ldots, x_{m}\right\}\right)=\emptyset \tag{7}
\end{equation*}
$$

Assume first that $d^{-}(z, E) \geq 1$. Then by Claim $1(\mathrm{i}), d^{+}(z, F)=0$. This together with (3) and (7) implies that $\mathcal{A}\left(\left\{z, x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$. Assume second that $d^{-}(z, E)=0$. Since $x_{l} z \notin \mathcal{A}(D)$, we obtain $\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\right.$ $\left.\left\{z, x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$. So, in both cases we have that the subdigraph $D-x_{l+1}$ is not strong, which contradicts that $D$ is 2 -strong.

Subcase 3.2. $b=l+1=m$.
Assume that $a \geq 2$. As mentioned above, either $x_{1} \rightarrow x_{a+1}$ or $x_{a+1} \rightarrow x_{1}$. Therefore, $C_{m+3}(z)=x_{1} x_{a+1} \ldots x_{m-1} y_{1} y_{2} x_{2} \ldots x_{a} x_{m} z x_{1}$ or $C_{m+2}(z)=x_{1} \ldots x_{a} x_{m} z x_{a+3} \ldots x_{m-1} y_{1} y_{2}$ $x_{a+1} x_{1}$. So, in both cases, we have a contradiction.

Assume next that $a=1$. Then from $d^{-}\left(z,\left\{x_{2}, x_{3}, \ldots, x_{m-1}\right\}\right)=0$ (by Claims 2(i) and $2(\mathrm{iv}))$ and $d^{-}(z) \geq 2$ it follows that $x_{1} \rightarrow z$. We know that $z \rightarrow\left\{x_{a+3}, \ldots, x_{l}\right\}$. Using this, it is not difficult to see that if $x_{i} \rightarrow x_{m}$ with $i \in[2, m-2]$, then for $i=2, C_{m+2}(z)=$ $x_{1} x_{2} x_{m} z x_{4} \ldots x_{m-1} y_{1} y_{2} x_{1}$, and for $i \in[3, m-2], C_{m+3}(z)=x_{1} x_{2} \ldots x_{i} x_{m} z x_{i+1} \ldots x_{m-1} y_{1}$ $y_{2} x_{1}$, a contradiction. We may, therefore, assume that

$$
\begin{equation*}
d^{-}\left(x_{m},\left\{x_{2}, x_{3}, \ldots, x_{m-2}\right\}\right)=0 \tag{8}
\end{equation*}
$$

Now we consider the vertex $x_{1}$. If $x_{j} \rightarrow x_{1}$ with $j \in[2, m-2]$, then for $j=2, C_{m+2}(z)=$ $x_{1} x_{m} z x_{4} \ldots x_{m-1} y_{1} y_{2} x_{2} x_{1}$, and for $j \in[3, m-2], C_{m+3}(z)=x_{1} x_{m} z x_{j+1} \ldots x_{m-1} y_{1} y_{2} x_{2} \ldots$ $x_{j} x_{1}$. Thus, in both cases, we have a contradiction. We may, therefore, assume that $d^{-}\left(x_{1},\left\{x_{2}, x_{3}, \ldots, x_{m-2}\right\}\right)=0$. This together with (3), (8) and $d^{-}\left(z,\left\{x_{2}, x_{3}, \ldots, x_{m-1}\right\}\right)=0$ implies that

$$
\mathcal{A}\left(\left\{x_{2}, x_{3}, \ldots, x_{m-2}\right\} \rightarrow Y \cup\left\{z, x_{1}, x_{m}\right\}\right)=\emptyset
$$

This means that $D-x_{m-1}$ is not strong, which contradicts that $D$ is 2 -strong.
Case 4. $a=l-2$. Taking into account Case 2 and the digraph duality, we may assume that $b \leq l+2$.

Subcase 4.1. $a=l-2$ and $b=l+2$. Then by Claim 2, $d\left(z,\left\{x_{l-1}, x_{l}, x_{l+1}\right\}\right)=0$. This together with (5) implies that

$$
\begin{gathered}
m-1 \leq d\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a}, x_{b}, x_{b+1}, \ldots, x_{m}\right\}\right) \leq a+m-b+2 \\
=m+l-2-l-2+2=m-2
\end{gathered}
$$

a contradiction.
Subcase 4.2. $a=l-2$ and $b=l+1$. Then by Claim $2, d\left(z,\left\{x_{l-1}, x_{l}\right\}\right)=0$.
Assume first that $m \geq l+2$. If there exist $i \in[l-1, l]$ and $j \in[l+2, m]$ such that $x_{i} \rightarrow x_{j}$, then $C(z)=x_{1} x_{2} \ldots x_{l-2} x_{l+1} \ldots x_{j-1} R\left(y_{1}, y_{2}\right) x_{i} x_{j} \ldots x_{m} z x_{1}$ is a cycle of length at least $m+2$, a contradiction. We may, therefore, assume that $\mathcal{A}\left(\left\{x_{l-1}, x_{l}\right\} \rightarrow\right.$ $\left.\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$. This together with (3), the minimality of $a$ and the maximality of $b$ implies that $\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \rightarrow\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$. Therefore, if $d^{-}(z, E)=0$, then $\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\left\{z, x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$, and if $d^{-}(z, E) \geq 1$, then $d^{+}(z, F)=0$ (Claim 1(i)) and $\mathcal{A}\left(\left\{z, x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$. Thus, in both cases, we have that $D-x_{l+1}$ is not strong, a contradiction.

Assume next that $m=l+1$. Then $a=l-2=m-3$. Let $a \geq 2$. From the minimality of $a$ it follows that $d^{-}\left(x_{m},\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right\}\right)=0$. If there exist $i \in$ [1,a-1] and $j \in[a+1, a+2]$ such that $x_{i} \rightarrow x_{j}$, then it is easy to see that $C(z)=$ $x_{1} x_{2} \ldots x_{i} x_{j} \ldots x_{m-1} R\left(y_{1}, y_{2}\right) x_{i+1} \ldots x_{a} x_{m} z x_{1}$ is a cycle of length at least $m+2$, a contradiction. We may, therefore, assume that $\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right\} \rightarrow\left\{x_{a+1}, x_{a+2}, x_{a+3}=x_{m}\right\}\right)=\emptyset$.

From this we have: if $d^{-}\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right)=0\right.$, then

$$
\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right\} \rightarrow Y \cup\left\{z, x_{a+1}, x_{a+2}, x_{a+3}\right\}\right)=\emptyset,
$$

if $d^{-}\left(z,\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right) \geq 1\right.$, then by Claim 1(i), $z x_{m} \notin \mathcal{A}(D)$ and

$$
\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{a-1}\right\} \cup\{z\} \rightarrow Y \cup\left\{x_{a+1}, x_{a+2}, x_{a+3}\right\}\right)=\emptyset .
$$

So, in both cases, we have that $D-x_{a}$ is not strong, which contradicts that $D$ is 2 -strong. Let now $a=1$. Then $m=4=b=l+1$ and $d\left(z,\left\{x_{2}, x_{3}\right\}\right)=0$. This together with $d(z, Y)=0, d^{+}(z) \geq 2$ and $d^{-}(z) \geq 2$ implies that $x_{1} \rightarrow z \rightarrow x_{4}$, which contradicts Claim 1(i).

Case 5. $a=l-1$. Taking into account Cases 3 and 4, we may assume that $b=l+1$. Then $d\left(z,\left\{x_{l}\right\}\right)=0$, and from (3), the minimality of $a$ and the maximality of $b$ it follows that

$$
\begin{align*}
& \mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l-1}\right\} \rightarrow Y \cup\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right) \\
= & \mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l-2}\right\} \rightarrow Y \cup\left\{x_{l+1}, x_{l+2}, \ldots, x_{m}\right\}\right)=\emptyset . \tag{9}
\end{align*}
$$

It is not difficult see that: if $x_{l} \rightarrow x_{j}$ with $j \in[l+2, m]$, then $C(z)=x_{1} x_{2} \ldots x_{l-1} x_{l+1} \ldots$ $x_{j-1} R\left(y_{1}, y_{2}\right) x_{l} x_{j} \ldots x_{m} z x_{1}$ is a cycle of length at least $m+3$, if $x_{i} \rightarrow x_{l}$ with $i \in[1, l-2]$, then $C(z)=x_{1} x_{2} \ldots x_{i} x_{l} R\left(y_{1}, y_{2}\right) x_{i+1} \ldots x_{l-1} x_{l+1} \ldots x_{m} z x_{1}$ is a cycle of length at least $m+3$. So, in both cases we have a contradiction. We may, therefore, assume that $d^{+}\left(x_{l},\left\{x_{l+2} x_{l+3}, \ldots, x_{m}\right\}\right)=d^{-}\left(x_{l},\left\{x_{1}, \ldots, x_{l-2}\right\}\right)=0$. Then by $(9)$,

$$
\begin{align*}
& \mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l-2}\right\} \rightarrow\left\{x_{l}, x_{l+1}, \ldots, x_{m}\right\}\right) \\
= & \mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \rightarrow\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset \tag{10}
\end{align*}
$$

Assume that $m \geq l+2$. If $d^{-}(z, E) \geq 1$, then $d^{+}(z, F)=0$ (Claim 1(i)). This together with (3), (10), $d\left(z,\left\{x_{l}\right\}\right)=0$ and $d(z, Y)=0$ implies that $\mathcal{A}\left(\left\{z, x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\right.$ $\left.\left\{x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset$, which in turn implies that $D-x_{l+1}$ is not strong, a contradiction. We may, therefore, assume that $d^{-}(z, E)=0$. Now it is not difficult to see that

$$
\mathcal{A}\left(\left\{x_{1}, x_{2}, \ldots, x_{l}\right\} \cup Y \rightarrow\left\{z, x_{l+2}, x_{l+3}, \ldots, x_{m}\right\}\right)=\emptyset
$$

This means that $D-x_{l+1}$ is not strong, a contradiction.
Assume now that $m=l+1$. By the digraph duality, we may assume that $a=l-1=1$. Hence, $b=l+1=m=3$. Then, since $d^{+}(z) \geq 2$ and $d^{-}(z) \geq 2, x_{1} \rightarrow z \rightarrow x_{m}$, which contradicts Claim 1(i). The discussion of Case 5 is completed. Lemma 5 is proved.

Now we are ready to prove the main result. For the convenience of the reader, we restate it here.

Theorem 9: Let $D$ be a 2-strong digraph of order $n \geq 8$ and $z$ be a fixed vertex in $\mathcal{V}(D)$. Suppose that for any vertex $x \in \mathcal{V}(D) \backslash\{z\}, d(x) \geq n, d(z) \geq n-4$, and $D$ contains a cycle of length $n-2$ passing through $z$. Then $D$ is Hamiltonian.

Proof. Suppose, on the contrary, that $D$ contains a cycle $C_{n-2}(z):=x_{1} x_{2} \ldots x_{n-2} x_{1}$ but it is not Hamiltonian. By Theorem 3 (or by Theorem 2), $d(z) \leq n-2$. Let $\left\{y_{1}, y_{2}\right\}=$ $\mathcal{V}(D) \backslash \mathcal{V}\left(C_{n-2}(z)\right)$. Since $z \in \mathcal{V}\left(C_{n-2}(z)\right)$, we have that $d\left(y_{i}\right) \geq n$. Using Lemma 1, it is easy to show that $D$ contains no $C_{n-1}(z), d\left(y_{1}\right)=d\left(y_{2}\right)=n, d\left(y_{1}, \mathcal{V}\left(C_{n-2}(z)\right)\right)=$
$d\left(y_{2}, \mathcal{V}\left(C_{n-2}(z)\right)\right)=n-2$ and $y_{1} \leftrightarrow y_{2}$. If $y_{1}$ or $y_{2}$ is adjacent to every vertex $x_{i}, i \in$ [1,n-2], then $D$ contains a cycle $C(z)$ of length at least $n-1$, a contradiction. We may, therefore, assume that $y_{1}$ and some vertex of $C_{n-2}(z)$ are not adjacent, say $x_{n-2}$. Then $d\left(y_{1},\left\{x_{1}, x_{2}, \ldots, x_{n-3}\right\}\right)=n-2$. Since $y_{1}$ cannot be inserted into $x_{1} x_{2} \ldots x_{n-3}$, using Lemma 2, we obtain that $x_{n-3} \rightarrow y_{1} \rightarrow x_{1}$. This together with $y_{1} \leftrightarrow y_{2}$ implies that $d\left(x_{n-2},\left\{y_{1}, y_{2}\right\}\right)=0$ (for otherwise, $D$ contains a cycle of length at least $n-1$ through $z$, which is a contradiction). Therefore, $d\left(y_{2},\left\{x_{1}, x_{2}, \ldots, x_{n-3}\right\}\right)=n-2$, and by Lemma 2, $x_{n-3} \rightarrow y_{2} \rightarrow x_{1}$. Then $C_{n-1}=x_{1} x_{2} \ldots x_{n-3} y_{1} y_{2} x_{1}$ is a cycle of length $n-1$. We know that $C_{n-1}$ does not contain the vertex $z$. Therefore, $z=x_{n-2}$. Thus, we have that the conditions of Lemma 5 hold. Therefore, $d(z) \leq n-5$, which contradicts that $d(z) \geq n-4$. The theorem is proved.

In [15], Overbeck-Larisch proved the following sufficient condition for a digraph to be Hamiltonian-connected.

Theorem 10: (Overbeck-Larisch [15]). Let $D$ be a 2-strong digraph of order $n \geq 3$ such that, for each two non-adjacent distinct vertices $x$, $y$ we have $d(x)+d(y) \geq 2 n+1$. Then for each two distinct vertices $u, v$ with $d^{+}(u)+d^{-}(v) \geq n+1$ there is a Hamiltonian $(u, v)$-path.

Let $D$ be a digraph of order $n \geq 3$ and let $u$ and $v$ be two distinct vertices in $\mathcal{V}(D)$. Follows Overbeck-Larisch [15], we define a new digraph $H_{D}(u, v)$ as follows: $\mathcal{V}\left(H_{D}(u, v)\right)=$ $\mathcal{V}(D-\{u, v\}) \cup\{z\}(z$ a new vertex $)$ and $\mathcal{A}\left(H_{D}(u, v)\right)=\mathcal{A}(D-\{u, v\}) \cup\left\{z y \mid y \in N_{D-v}^{+}(u)\right\} \cup$ $\left\{y z \mid y \in N_{D-u}^{-}(v)\right\}$.

Now, using Theorem 7, we will prove the following theorem, which is an analogue of the Overbeck-Larisch theorem.

Theorem 11: Let $D$ be a 3-strong digraph of order $n+1 \geq 10$ with minimum degree at least $n+2$. If for two distinct vertices $u, v, d_{D}^{+}(u)+d_{D}^{-}(v) \geq n-2$ or $d_{D}^{+}(u)+d_{D}^{-}(v) \geq n-4$ with $u v \notin \mathcal{A}(\mathcal{D})$, then there is a Hamiltonian ( $u, v$ )-path in $D$.

Proof. Let $D$ be a 3 -strong digraph of order $n+1 \geq 10$ and let $u, v$ be two distinct vertices in $\mathcal{V}(D)$. Suppose that $D$ and $u, v$ satisfy the degree conditions of the theorem. Now we consider the digraph $H:=H_{D}(u, v)$ of order $n \geq 9$. By an easy computation, we obtain that the minimum degree of $H$ is at least $n-4$, and $H$ has $n-1$ vertices of degrees at least $n$. Moreover, we know that $H$ is 2 -strong (see [10]). Thus, the digraph $H$ satisfies the conditions of Theorem 7. Therefore, $H$ is Hamiltonian, which in turn implies that in $D$ there is a Hamiltonian $(u, v)$-path.

## 5. Conclusion

For Hamiltonicity of a graph $G$ (undirected graph), there are numerous sufficient conditions in terms of the number $k(G)$ of connectivity, where $k(G) \geq 3$ (recall that for a graph $G$ to be Hamiltonian, $k(G) \geq 2$ is a necessary condition) and the minimum degree $\delta(G)$ (or the sum of degrees of some vertices with certain properties), see the survey papers by Gould, e.g. [16]. This is not the case for the general digraphs. In [17], the author proved that: For every pair of integers $k \geq 2$ and $n \geq 4 k+1$ (respectively, $n=4 k+1$ ), there exists a $k$-strong ( $n-1$ )-regular (respectively, with minimum degree at least $n-1$ and with minimum semi-degrees at least $2 k-1=(n-3) / 2$ ) a non-Hamiltonian digraph of order $n$. In [1] (Page

253 ), it was showed that there is no $k$ such that every $k$-strong multipartite tournament with a cycle factor has Hamiltonian cycle.

Based on the evidence from Theorem 9, we raise the following conjecture, the truth of which in the case $k=0$ follows from Theorem 9 .

Conjecture 2: Let $D$ be a 2-strong digraph of order $n$ and $z$ be a fixed vertex in $\mathcal{V}(\mathcal{D})$. Suppose that for any vertex $x \in \mathcal{V}(D) \backslash\{z\}, d(x) \geq n+k$ and $d(z) \geq n-k-4$, where $k \geq 0$ is an integer. Then $D$ is Hamiltonian.

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<br><br> e-mail: samdarbin@iiap.sci.am

## Uựnఛnnư









# Об одном расширении теоремы Гуйя-Ури 

Самвел X. Дарбинян<br>Институт проблем информатики и автоматизации НАН РА<br>e-mail: samdarbin@iiap.sci.am


#### Abstract

Аннотация В настоящей работе доказана следующая теорема. Теорема. Пусть $D$ есть 2 -сильно связный $n \geq 8$ вершинный орграф, в котором $n-1$ вершин имеют степень не меньше чем $n$, а вершина $z$ имеет степень не меньше чем $n-4$. Если $D$ содержит контур длины $n-2$, которий содержит вершину $z$, то $D$ содержит гамильтонов контур.

Ключевые слова: орграф, гамильтонов контур, 2-сильно, гамильтоновосвязныий.


# Comparison of Model-Free Algorithms For Clustering GARCH Processes 

Garik L. Adamyan<br>Yerevan State University<br>e-mail: garik.adamyan@ysu.am


#### Abstract

In this paper, we evaluate several model-free algorithms for clustering time series datasets generated by GARCH processes. In extensive experiments, we generate synthetic datasets in different scenarios. Then, we compare K-Means (for Euclidian and dynamic time warping distance), K-Shape, and Kernel K-Means models with different clustering metrics. Several experiments show that the K-Means model with dynamic time warping distance archives comparably better results. However, the considered models have significant shortcomings in improving the clustering accuracy when the amount of information (the minimum length of the time series) increases, and in performing accurate clustering when data is unbalanced or clusters are overlapping.


Keywords: Time series clustering, GARCH process, dynamic time warping, K-Means, K-Shape.
Article info: Received 02 May 2022; received in revised form 20 July 2022; accepted 29 September 2022.

## 1. Introduction

Time series clustering has been used in diverse scientific disciplines to discover patterns and extract valuable information from complex and massive datasets. These algorithms have a wide range of applications in many research areas, for instance, in finance, biology, and robotics [1].

Time series clustering approaches can be classified as feature-based, shape-based, and model-based [1]. It is noteworthy that these methods are based on dissimilarity measures on time series data, according to which the time series data points are grouped by some clustering method (for instance, PAM).

In general, shape-based methods use linear and non-linear transformations to align time series samples and calculate dissimilarity measures on aligned samples. Additionally, shape-based algorithms process the time series data directly without making any statistical assumptions about the underlying data generating processes. On the contrary, model-based methods make statistical assumptions on time series generating processes. In general, modelbased approaches assume that time series samples are generated from specific models (for
instance, ARIMA [2], Mixtures of ARIMAs [3]). Time series samples are transformed into fitted models, and then a suitable distance and a clustering algorithm are applied to the estimated model parameters.

Although several benchmarking results on different real-world datasets for nonparametric clustering methods can be found in ([4], [5], [6]), the comparison of nonparametric clustering methods on time series data generated from GARCH processes is not well studied. In this paper, we are interested in non-parametric models evaluation of time series data generated from the well-known GARCH process, which is the actual choice for modeling the volatility of returns on financial assets. We simulate multiple GARCH models with different data generating scenarios and compare several non-parametric time series clustering models.

Motivated by [4], for comparison we choose well-known partition-based time series clustering models: K-Means, K-Means with dynamic time warping and DTW barycenter averaging, K-Shape and Kernel K-Means models. Furthermore, we can find open-source implementations of these algorithms [7].

Although the main focus in the field of time series clustering comparison remains clustering accuracy metrics, in this work we also explore a number of other challenges of model-free methods. In particular, we study the ability of the above-mentioned modelfree methods to cluster GARCH processes with imbalanced, overlapping clusters and also examine the impact of increasing information on clustering accuracy.

## 2. Related Work

In time series analysis research, benchmarking and numerical comparison have been recognized as integral steps to justify theoretical results. The importance of numerical comparison is emphasized in [8], where the authors reimplemented many time-series classification algorithms and compared them in 50 real-world datasets. The authors note that most reported methods have insignificant improvements regarding the variance of the evaluation metrics. This empirical evidence reclaimed the statement of the importance of the time series benchmark datasets and the empirical evaluation of the suggested methods.

Among the works that compare time series clustering models based on real-world datasets, we can mention ([4], [5], [6]) works. In [4], authors compare several partition, density, and hierarchical clustering methods to cluster all time series datasets available in the University of California Riverside (UCR) archive [9]. They conclude that the overall performance of the eight compared algorithms is quite similar with high dependence on the evaluation dataset.

The method of comparing time series clustering algorithms with synthetic, generated datasets also attracts a lot of attention among scholars. In addition to the actual clusters being known, this comparison method gives additional flexibility to examining the behavior of algorithms in different situations. In particular, scholars discussed the difference between stationary and non-stationary time series [10], the presence of noise in time series samples [11], the presence of noise clusters in time series dataset [11].

## 3. Clusters of GARCH

The GARCH process is introduced in [12] for statistical modeling of the volatility of returns on financial assets. The GARCH model has many extensions such as asymmetric GARCH [13], threshold GARCH [14]. The GARCH $(\mathrm{p}, \mathrm{q})$ model is defined as follows:

$$
\begin{gathered}
y_{t}=\mu_{t}+\epsilon_{t} \\
\epsilon_{t}=\sigma_{t} e_{t}, \quad \text { where } \quad e_{t} \quad i . i . d \quad E\left(e_{t}\right)=0, \operatorname{var}\left(e_{t}\right)=1 \\
\sigma_{t}^{2}=\omega+\sum_{i=1}^{p} \alpha_{i} \epsilon_{t-i}^{2}+\sum_{j=1}^{q} \beta_{j} \sigma_{t-j}^{2}
\end{gathered}
$$

where

$$
\begin{gathered}
\omega>0 \\
\alpha_{i} \geq 0, i=1,2, \ldots, p, \\
\beta_{j} \geq 0, i=1,2, \ldots, q .
\end{gathered}
$$

The $\operatorname{GARCH}(\mathrm{p}, \mathrm{q})$ model admits a strictly stationary solution with a finite variance if and only if

$$
\begin{equation*}
\sum_{i=1}^{p} \alpha_{i}+\sum_{j=1}^{q} \beta_{j}<1 \tag{1}
\end{equation*}
$$

Moreover, this strictly stationary solution is also unique. [15]
For the evaluation of non-parametric models, we chose constant zero mean specification for the GARCH model because it is advised to standardize input data prior to clustering. In addition, we choose the innovations $e_{t}$ as standard Gaussian innovations. So $\mu_{t}=0$ and $e_{t} \sim \mathcal{N}(0,1)$.

In order to measure the clustering accuracy, we need to define the ground truth clusters of GARCH processes. Let $N, K, T \in \mathbb{N}$ where $K$ is the number of clusters, $N$ is the number of samples and $T$ is the time sample size of each series. In this paper, we consider samples with a fixed time size $T$, because some of the models (ex. KM-E) support samples with fixed length. We denote by $P^{i}=\left(\omega, \alpha_{1}, \alpha_{2}, \ldots, \alpha_{p_{i}}, \beta_{1}, \beta_{2}, \ldots, \beta_{q_{i}}\right)$ the vector of all parameters for the given $\operatorname{GARCH}\left(p_{i}, q_{i}\right)$ model.

Let $\left\{P^{i}\right\}_{i=1}^{K}$ be a family of GARCH process parameters, where $K$ is a number of clusters. Assume that each $P^{i}(i=1,2, \ldots, K)$ is unique and all the parameters satisfy (1) in order to provide a strict stationary solution of the corresponding model. We are given $N$ samples of time series $Y_{i}=\left\{y_{t}^{i}\right\}_{i=1}^{T}$, where each sample is generated from one of the $K$ GARCH processes.

Definition 1. We say that $Y_{i}$ and $Y_{j}$ samples are from the same cluster if they are generated from the same GARCH process.

In other words, a cluster of GARCH processes is a set of samples that are generated with the same parameters. The uniqueness of the parameters $P^{i}$ and Definition 1 imply that the given sample belongs to exactly one cluster.

## 4. Evaluation Models

For evaluation, we choose well-known non-parametric time series clustering models such as K-Means with Euclidean (KM-E) and dynamic time warping metrics (KM-DTW), K-Shape, and Kernel K-Means with Fast Global Alignment Kernel (KKM-GAK) models. KM-E uses Euclidean distance, for cluster assignment and means averaging for the barycenter (centroid) computation. It is known that the Euclidean distance metric is not the most accurate metric for measuring time series similarities. Firstly, to use Euclidean distance, we need to take into account the order of elements in the time series; secondly, the Euclidean distance does not consider a phase shift between two curves or a length difference between the series. In this paper, we consider this model for comparison with more complex approaches.

KM-DTW uses dynamic time warping [16] for cluster assignment and DTW barycenter averaging (DBA) [17] algorithm for averaging time series within the same cluster.
k -Shape [18] is a partitional clustering algorithm that relies on an iterative refinement procedure similar to the one used in K-Means. To measure the distance between time series, K-Shape uses a normalized version of the cross-correlation measure to consider the shapes of time series while comparing them. During the iterative procedure, this model minimizes the sum of squared distances between the sequences of time series.

Kernel K-Means[19] is an alternative clustering algorithm that uses kernel functions as a nonlinear mapping from the input space to a higher dimensional space. By using kernels, Kernel K-Means can separate clusters in higher dimensional space, even if the input data is not non-linearly separable in the input space. For treating time series data, practitioners usually used Global Alignment Kernels [20]. We will refer to this algorithm KKM-GAK.

The problem is to generate synthetic datasets and evaluate non-parametric models for clustering time series processes generated by the GARCH model.

## 5. Assessment Metrics

In practice, the use of clustering methods is due to working with unlabeled datasets. As a result, we can find evaluation metrics that can evaluate clustering models without having labeled data. These types of metrics are called internal. By the method of our data generating process, we can use external measures, which assume that ground truth labels are available. Examples of this type of metrics are the Rand Index (RI) [21], the Adjusted Rand Index (ARI) [22], the Adjusted Mutual Information (AMI)[23].

Following the evaluation made in [4] in our study, we choose the Adjusted Rand Index, because the values of this metric are consistently low for random cluster assignments and do not depend on the number of clusters.

## 6. Experiments

To evaluate non-parametric models, we simulate random datasets with different setups. In the first experiment, we measure the ability of the models of clustering different numbers of clusters. For this purpose, we generate datasets for $2,4,8$, and 10 clusters, respectively. For each number of clusters, we generate random parameter families, which satisfy (1) for guaranteeing a unique and stationary solution of processes. For the purpose of generating a family of parameters, we constrain the maximum length of $p$ and $q$ by 5 . This constraint is inherited from the common choice of GARCH models with fewer parameters. For every
parameter vector $P^{i}$ (cluster), we generate samples for the given cluster and separate them into training and testing parts ( $30 \%$ testing) and repeat this process for averaging purposes. In Table 1, we present the results of the first experiment evaluated with the AMI metric. We can see that the KM-DTW model outperforms other models. In the second experiment,

Table 1: AMI score for different $N$ clusters

| $N$ clusters | KM-E | KM-DTW | k-Shape | KKM-GAK |
| :---: | :---: | :---: | :---: | :---: |
| 2 | $0.003+-0.001$ | $0.325+-0.403$ | $0.004+-0.009$ | $0.003+-0.002$ |
| 4 | $0.004+-0.001$ | $0.463+-0.129$ | $0.02+-0.007$ | $0.002+-0.001$ |
| 6 | $0.018+-0.016$ | $0.578+-0.151$ | $0.043+-0.021$ | $0.001+-0.0005$ |
| 8 | $0.006+-0.003$ | $0.498+-0.077$ | $0.005+-0.011$ | $0.001+-0.0005$ |
| 10 | $0.005+-0.01$ | $0.624+-0.03$ | $0.062+-0.022$ | $0.0001+-0.00005$ |

we measure the clustering quality in scenarios when the amount of information increases. We generate datasets with 5 clusters and 100 samples in each cluster. We set $T=1000$ and consider 5 intervals on the time axis. We train and evaluate models in the first interval and consequently add information. From the second experiment, we can see that the KM-DTW model outperforms other models, but we do not observe increased accuracy as a result of adding information. There is a significant increase in the accuracy of the KM-DTW model when the number of samples increases from 200 to 400 , but further increases in the number of samples do not improve the accuracy of the model. The K-Shape model also shows a slight improvement in accuracy when the number of samples increases from 800 to 1000 . Given that model-based methods rely on ML/Quasy ML estimates of the parameters of GARCH models and also the asymptotic properties of these estimates, this experiment may suggest that model-based methods have the potential to increase clustering accuracy as information increases. The results of the second experiment are displayed in Fig. 1.


Fig. 1. AMI for different time intervals.

Fig. 2 shows the results of the third experiment. In this experiment, we measure the ability of the KM-DTW model to cluster an imbalanced dataset. For the fairness of the experiment, we generate time series samples with the $\operatorname{GARCH}(1,1)$ process and ensure that parameters satisfy (1). In addition, we constrain the $L_{2}$ norm of generated parameters to obtain non-overlapping clusters. We generate a dataset with different sample ratios and increase the ratio to 1 . In the figure, we can observe that the best model for other experiments KM-DTW is dependent on cluster imbalance. This experiment shows that the claim made in [24] that centroid-based methods should be adapted to unbalanced scenarios also holds in the domain of time series clustering.


Fig. 2. Results for clustering imbalanced dataset.
Moreover, we measure the effect of the $L_{2}$ norm of generated parameters in clustering accuracy. We generate parameters for $\operatorname{GARCH}(1,1)$ process so that the parameters satisfy the current restriction on the $L_{2}$ norm. Throughout the experiment, we increase the bounds of the $L_{2}$ norm. During each step, we generate a balanced dataset with $T=500, C=2$, and 100 samples per cluster. We train models ten times for averaging purposes. We can observe that the KM-DTW model depends on clusters overlapping and increasing the bounds of parameters $L_{2}$ norm results in improvement of AMI. This problem is directly related to the ability of the similarity measure used in the KM-DTW algorithm to distinguish realizations of the GARCH process with parameters that are close to each other with the L2 norm.

## 7. Conclusion and Future Work

In this work, several non-parametric clustering algorithms for clustering time series datasets generated by GARCH processes are evaluated. We generate multiple datasets and conduct multiple experiments to evaluate the K-Means (with Euclidean and dynamic time warping distance), K-Shape, and Kernel K-Means models. In the first experiment, we evaluate the ability of models to cluster different numbers of clusters. The results of the first experiment


Fig. 3. GARCH parameters vector $L_{2}$ norm versus AMI score.
are displayed in Table 1. In the second experiment, we measure the clustering quality in the scenarios when the amount of information increases. We generate a dataset with 1000 time length and increase the information set. The results of the second experiment are shown in Fig. 1. During both experiments, the KM-DTW model shows better results. In the third experiment, we measure the ability of the KM-DTW model to cluster imbalanced datasets by generating multiple datasets with imbalanced samples in the cluster. The results are provided in Fig. 2. In the fourth experiment, we measure the ability of the KM-DTW model to cluster overlapping clusters. We constrain the norm of the parameters of the $\operatorname{GARCH}(1,1)$ model and evaluate the KM-DTW model. The experiment shows that KM-DTW is highly dependent on the norm of the generated parameters. The results of the fourth experiment are shown in Fig. 3.

We hope that our findings can motivate scholars to examine the discussed issues related to clustering accuracy, cluster overlapping, and available information effect. We think that already designed GARCH-based clustering methods have the potential to overcome these problems, so it is important to conduct similar experiments to show this. Moreover, as a direct application of our findings, it is worth applying clustering algorithms to the real-world financial dataset.

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# GARCH wnngtuaitinh limuntinhquaghujh huwiwn unntilitinhg uGiluru wıqn 

Yuphl L. Unuưjua<br><br>e-mail: garik.adamyan@ysu.am

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# Сравнение безмодельных алгоритмов кластеризации GARCH-процессов 

Гарик $\Lambda$. Адамян<br>Ереванский государственный университет, Ереван, Армения<br>e-mail: garik.adamyan@ysu.am

## Аннотация

В этой статье мы оцениваем некоторые безмодельные алгоритмы кластеризации наборов данных временных рядов, сгенерированных GARCH процессами. В обширных экспериментах мы генерируем синтетические наборы данных для различных сценариях. Затем мы сравниваем модели K-Means (с метриками евклидовой и динамической трансформации временной шкалы), модели KShape и Kernel K-Means с различными метриками кластеризации. Несколько экспериментов показывают, что модель K-Means с метрикой динамической трансформации временной шкалы дает сравнительно лучшие результаты. Однако рассмотренные модели имеют существенные недостатки в повышении точности кластеризации при увеличении количества информации (минимальной длины временного ряда), а также при несбалансированности данных или перекрытии кластеров.

Ключевые слова: кластеризация временных рядов, процесс GARCH, динамическая деформация времени, K-Means, K-Shape.

# A Brief Comparison Between White Box, Targeted Adversarial Attacks in Deep Neural Networks 

Grigor V. Bezirganyan and Henrik T. Sergoyan<br>Department of Mathematics, Technical University of Munich, Muinch, German<br>e-mail: grigor.bezirganyan@tum.de, henrik.sergoyan@tum.de


#### Abstract

Today, neural networks are used in various domains, in most of which it is critical to have reliable and correct output. This is why adversarial attacks make deep neural networks less reliable to be used in safety-critical areas. Hence, it is important to study the potential attack methods to be able to develop much more robust networks. In this paper, we review four white box, targeted adversarial attacks, and compare them in terms of their misclassification rate, targeted misclassification rate, attack duration, and imperceptibility. Our goal is to find the attack(s), which would be efficient, generate adversarial samples with small perturbations, and be undetectable to the human eye.


Keywords: Adversarial Attacks, Robustness, Machine Learning, Deep Learning.
Article info: Received 26 April 2022; received in revised form 4 July 2022; accepted 29 July 2022.

## 1. Introduction

Nowadays, deep neural networks are becoming more and more popular to solve problems in various domains, including safety-critical areas such as medicine, self-driving cars, etc. Unfortunately, techniques to fool deep learning models have recently come out to provide incorrect outputs [1]. Particularly, in the image classification domain, an attacker can create an altered image, which will be misclassified by a model but will be classified correctly by a human. This altered image is often referred to as an adversarial example, and this process as an adversarial attack. To be protected against such attacks, researchers try to create methods to make the models more robust against such perturbations. Studying adversarial attacks and their potential helps us develop better countermeasures against them.

In this paper, we will discuss some of the adversarial algorithms and test them against an image classification model. We then compare the results of the experiments in terms of their misclassification rate, targeted misclassification rate, attack duration, and imperceptibility.

### 1.1 Definitions and Notations

### 1.1.1 Poisoning Attacks vs Evasion Attacks

In poisoning attacks, the attacker tries to insert fake samples (i.e., data samples with wrong labels) into the training dataset, which will make the model learn on those fake samples and output wrong results. This kind of attack is possible when the attacker has the means to import those fake samples into the training set. In contrast, in evasion attacks, the attacker does not need access to the dataset. In this case, the attacker creates adversarial samples, which are similar and hard to distinguish by a human from the original samples but are misclassified by the trained model.

### 1.1.2 Attacker's Knowledge of the Model

Based on how much information the attacker has about the model, attacks can be classified into white-box, black-box, and gray-box attacks. In the white box scenario, the attacker has full knowledge about the model architecture and uses this knowledge to generate adversarial examples. In contrast, in the black-box setup, the attacker does not know the architecture. Instead, the attacker observes the output of the model from the given input. Some of the attacks assume access to the soft labels (i.e., probability or likelihood score of belonging to a class), while others try to generate examples based on only hard labels (i.e., class labels without the score). In the gray-box setting, the attacker has an access to the original model and trains a generative model on it. When the generative model is ready, the attacker uses that model to generate adversarial samples. Hence, the original model is no more needed. Recently, in [2] another category was introduced, called no-box attacks. In contrast to black-box attacks, the attacker cannot query the model, instead, he has a small number of samples from the same domain as the victim. The authors train an auto-encoder on those samples and then generate the adversarial examples using the features learned from the auto-encoder.

### 1.1.3 Targeted vs Non-Targeted Attacks

In the targeted attack, the attacker tries to misclassify the given sample into a specific target label. In contrast, in non-targeted attacks, the attacker tries to classify the sample into any other class.

### 1.2 Our Goal and Contribution

In this paper, we try to overview some of the adversarial attack techniques and, running experiments in the same setting, compare them based on:

- Misclassification: What percentage of the adversarial samples were misclassified
- Targeted Misclassification: What percentage of the adversarial samples were successfully misclassified to the target class
- Imperceptibility: How much the adversarial example looks like the original image
- Duration of the attack: How long it takes to generate an adversarial example

In this paper, we will concentrate only on white-box and target attacks. In particular, we will discuss and experiment with the Fast Gradient Sign Method [1], Projected Gradient Descent [3], AutoPGD [4], and FW + Dual LMO [5]. We chose these attack methods as FGSM is one of the first and simplest methods, which is still popular today. PGD is the most popular, as even many new state-of-the-art methods are modified versions of the PGD attack. AutoPGD, being one of those variations, achieves state-of-the-art results according to the authors. And while these attacks use $\ell_{p}$ norms, we also chose FW + Dual LMO as an example of an attack that uses another norm (Wasserstain norm in this case).

## 2. Attack Mechanisms

In this section, we will briefly overview the attacks, which will be used for experimentation further in the paper.

In our attacks, we are given a set of input images $x \in \mathbb{R}^{n \times n}$, and our goal is to craft an adversarial example $x^{\prime} \in \mathbb{R}^{n \times n}$ that will be misclassified by the deep learning model $F$ : $\mathbb{R}^{n \times n} \rightarrow \mathbb{N}$. Since we are discussing targeted attacks, we want to misclassify the adversarial sample into our desired target class $t \in \mathbb{N}$ instead of the original class $y \in \mathbb{N}$. Furthermore, the perturbation we add to the image should be as small as possible, not to be detected by a human. So, we can formulate the problem in the following way: Given a Neural Network $F: \mathbb{R}^{n \times n} \rightarrow \mathbb{N}$, input image $x \in \mathbb{R}^{n \times n}$ with a label $y \in \mathbb{N}$, a distance function $\|\cdot\|$ and a perturbation budget $\epsilon \in \mathbb{R}$ find an $x^{\prime} \in \mathbb{R}$ such that

$$
\begin{array}{ll} 
& F\left(x^{\prime}\right)=t \neq y \\
\text { s.t. } & \left\|x^{\prime}-x\right\| \leq \epsilon . \tag{1}
\end{array}
$$

In our case, the distance functions will be $l_{1}, l_{2}, l_{\infty}$ distances or the Wasserstein distance.

### 2.1 Fast Gradient Sign Method (FGSM)

Since we can access the gradients of the network in the white-box setting, what most of the gradient-based attacks do, is to fix the network weight and maximize the loss by updating the image. For that, they add a small perturbation $\eta \in \mathbb{R}^{n \times n}$ to the original image:

$$
x^{\prime}=x+\eta
$$

The most efficient way to maximize the loss would be to add noise in the same direction as the gradients. [1] introduced an attack method, where they do exactly that: add a perturbation in a direction that will increase the loss function $\mathcal{L}$ between the adversarial example and the original label

$$
\begin{equation*}
x^{\prime}=x+\epsilon \cdot \operatorname{sign}\left(\nabla_{x} \mathcal{L}(\theta, x, y)\right) . \tag{2}
\end{equation*}
$$

We can see that in this way the maximum allowed perturbation is added, while still being in the $\epsilon$ ball.

For a targeted setting, the update step will become:

$$
x^{\prime}=x-\epsilon \cdot \operatorname{sign}\left(\nabla_{x} \mathcal{L}(\theta, x, t)\right)
$$

in other words, a perturbation is added to minimize the loss between the adversarial sample and the target class $t$.

### 2.2 Projected Gradient Descent

The Projected Gradient Descent attack (PGD) or Basic Iterative Method (BIM) was introduced in [3], where they transformed the FGSM [1] one-step attack into an iterative one by performing the update step (2) multiple times with a small step size $\alpha \in \mathbb{R}^{n \times n}$. This will work better, as the FGSM adds the maximum allowed perturbation, but does not guarantee to maximize the loss within the allowed $\epsilon$-ball. In contrast, in an iterative approach, the algorithm is more likely to find the maxima. To ensure that the adversarial sample remains in the $\epsilon$ neighborhood, PGD projects the sample back to the $\epsilon$ ball after each update step. In other words, it performs projected gradient descent (or ascent) on the input sample. The update steps for targeted and untargeted attacks will be as follows:

$$
\begin{align*}
& x^{(i+1)}=\Pi_{\epsilon}\left(x^{(i)}+\alpha \cdot \operatorname{sign}\left(\nabla_{x^{(i)}} \mathcal{L}\left(\theta, x^{(i)}, y\right)\right)\right)  \tag{3}\\
& x^{(i+1)}=\Pi_{\epsilon}\left(x^{(i)}-\alpha \cdot \operatorname{sign}\left(\nabla_{x^{(i)}} \mathcal{L}\left(\theta, x^{(i)}, t\right)\right)\right) \tag{4}
\end{align*}
$$

So, the attacker tries to find a perturbation that either finds the maximum loss between $x^{\prime}$ and $y(3)$ (untargeted attack), or the minimum loss between $x^{\prime}$ and $t$ (4) (targeted attack).

### 2.3 Auto-Projected Gradient Descent

It has recently been suggested [4] that the Cross-Entropy loss and the fixed step size of the PGD attack [3] may be two reasons for its potential failure. They propose an alternative loss function and a new gradient-based method, Auto-PGD, which does not require a fixed step size.

They divide their method into two phases: an exploration phase and an exploitation phase. During the exploration phase, they search for good initial points, while in the exploitation phase, they try to maximize the accumulated knowledge. The step size value depends on the trend of optimization. If the objective function decreases rapidly, then the step size does not need to be changed, otherwise, if it decreases slowly, the step size is reduced.

### 2.4 Wasserstein Attack

The Wasserstein adversarial attack was introduced in [6]. Here they proposed to use the Wasserstein distance instead of the commonly used $\ell_{p}$ distances. For images, the Wasserstein distance can be seen as the cost of redistributing pixel mass. For example, while rotations change $\ell_{p}$ norms dramatically, they only slightly change the Wasserstein distance.

So, what their algorithm does, is to do a PGD attack [3], but instead of projecting on an $\ell_{p}$ norm, they project on the Wasserstein ball. However, since the projection onto the Wasserstein ball is computationally expensive, they make an approximation by performing modified Sinkhorn iterations [7].
[5] improved the algorithm by introducing an exact but still efficient projection operator. They also introduce an adversary generating method based on the Frank-Wolfe [8] method equipped with a suitable linear minimization oracle and show that it works very fast for Wasserstein constraints.

In this paper, we will use that Frank-Wolfe method (FW + Dual LMO) for the experiments.

## 3. Experiments

### 3.1 Goal

In this experiment, our goal is to run FGSM [1], PDG [3], AutoPGD [4], and FW + Dual LMO [5] attacks on the same environment and compare them in terms of misclassification, targeted misclassification, attack duration, and imperceptibility.

### 3.2 Setup

We are performing our experiments on a pre-trained ResNet-18 [9] classifier on the CIFAR10 dataset [10], with initial $92.4 \%$ accuracy on the test set. We generate the adversarial examples on a server with an Nvidia GeForce GTX 1080-Ti GPU.

We use the Adversarial Robustness Toolkit (ART) [11] for FGSM [1] and PGD [3] and AutoPGD [4] attacks, and the original implementation by the authors for FW + Dual LMO [5]. We run each of the adversarial attacks with a set of epsilon values in $\epsilon \in(0,0.5]$ and for all target classes. We use $\ell_{p}$ norms for FGSM, PGD, and AutoPGD, and we use the Wasserstein distance for the FW + Dual LMO. All the other hyper-parameters are left to their default values. For the FW + Dual LMO, in the original implementation, there was no option for targeted attacks. Hence, we modified their implementation and added the option for target attacks. For that we converted the problem:

$$
\begin{aligned}
& \operatorname{maximize} \quad \mathcal{L}\left(F\left(x^{\prime}\right), y\right) \\
& \text { subject to }\left\|x^{\prime}-x\right\| \leq \epsilon
\end{aligned}
$$

to

$$
\begin{aligned}
& \text { minimize } \quad \mathcal{L}\left(F\left(x^{\prime}\right), t\right) \\
& \text { subject to }\left\|x^{\prime}-x\right\| \leq \epsilon
\end{aligned}
$$

We log the duration of the attack, the misclassification rate, and the targeted misclassification rate for later comparison. The source code for the experiment can be found https://github.com/bezirganyan/adversarial ${ }_{a}$ renahere.

## 4. Results

### 4.1 Targeted Misclassification and Misclassification Rate

We first look at the average misclassification and targeted misclassification scores that each of our models was able to achieve for some $\epsilon \in(0,0.5]$. In Table 1 , we can see average misclassification and targeted misclassification rates for the best epsilon of each attack. As we can see from the $\ell_{p}$ attacks, the $\ell_{\infty}$ norm yields the highest scores in our setup. Hence, from now on we will use the $\ell_{\infty}$ norm for further comparisons. Note that this does not mean that the $\ell_{\infty}$ norm is better since we could get similar scores and similar perturbations for higher $\epsilon$ values under other norms, as the $\ell_{\infty}$ attack will add a higher amount of perturbation under the same epsilon.

Furthermore, we can see that from the $\ell_{p}$ attacks in terms of targeted misclassification rate, the PGD, and AutoPGD attacks yield very high scores leaving the FGSM attack behind with a huge margin. In general, PGD and AutoPGD attacks behave almost identically in
our experiments. We hypothesize that this is because we are testing on an undefended model, on which they both reach their maximum potential limit. The developers of the ART framework confirmed that on their tests on defended models in an untargeted setting, AutoPGD behaved slightly better. We, hence, plan to test and compare the models on a defended model in our future work. In Fig. 1, we can see the Misclassification and Targeted misclassification rates of the attacks for different epsilons and under the $\ell_{\infty}$ norm. We can see that in terms of misclassification and targeted misclassification rates the PGD and AutoPGD attack perform best within the $\ell_{p}$ attacks by having around $90 \%$ misclassification rate even for very small epsilon.


Fig. 1. Average misclassification and targeted misclassification rates for different $\epsilon$ values under $\ell_{\infty}$ and Wasserstein (FW) norms.

Furthermore, we can see that for the FGSM attack, the targeted misclassification does not increase monotonically. The reason for this can be that since the FGSM is not an iterative algorithm and performs just one step, it overshoots when the epsilon is too big and misses the target class.

The FW+Dual LMO attack performs best in terms of both misclassification and targeted misclassification rates. Nevertheless, we cannot compare the amount of perturbation under $\ell_{\infty}$ and Wasserstein norms, since they imply different amounts of changes to the image. Hence, we will need to combine these results with the visual ones to be able to make a fair comparison.

### 4.2 Duration

In Table 2, we can see the time duration needed to generate an adversarial example. Being a simple one-step attack, FGSM leads the competition followed by the PGD and AutoPGD

Table 1: Average misclassification and average targeted misclassification rates for different norms

| attack | norm | miscl | targ. miscl. |
| :---: | :---: | :---: | :---: |
| AutoPGD | $\ell_{1}$ | 0.0832 | 0.1100 |
| PGD | $\ell_{1}$ | 0.0810 | 0.1086 |
| FGSM | $\ell_{1}$ | 0.0879 | 0.1116 |
| AutoPGD | $\ell_{2}$ | 0.8968 | 0.9977 |
| FGSM | $\ell_{2}$ | 0.6157 | 0.3914 |
| PGD | $\ell_{2}$ | 0.8927 | 0.9925 |
| AutoPGD | $\ell_{\infty}$ | 0.9000 | 1.0000 |
| FGSM | $\ell_{\infty}$ | 0.9149 | 0.5515 |
| PGD | $\ell_{\infty}$ | 0.9022 | 1.0000 |
| FW | was | 0.9000 | 1.0000 |

attacks. PGD, which performs much better than FGSM in terms of targeted misclassification rate, is around 71 times slower. The slowest is the FW + Dual LMO attack, which performs around 400 times slower than the FGSM attack.

### 4.3 Duration

In Table 2, we can see the time duration needed to generate an adversarial example. Being a simple one-step attack, FGSM leads the competition followed by the PGD and AutoPGD attacks. PGD, which performs much better than FGSM in terms of targeted misclassification rate, is around 71 times slower. The slowest is the FW + Dual LMO attack, which performs around 400 times slower than the FGSM attack.

Table 2: Duration of generating an adversarial example in seconds.

| FGSM | PGD | AutoPGD | FW+Dual LMO |
| :--- | :--- | :--- | :--- |
| 0.7 | 50 | 87 | 338 |

### 4.4 Imperceptibility

One of the most important aspects of Adversarial attacks is that they should be undetected by the human eye. Hence, in this section, we study how detectable are the adversarial samples generated by the attacks. To visualize the results, we chose the smallest $\epsilon$ for each of our attacks, under which our model showed at least $80 \%$ misclassification. You can see the visualizations in the Figures 2 and 3. We can see that in the examples generated by the FGSM attack, although the original image is still well visible, the perturbation is easily detectable to us. For PGD, AutoPGD, and FW + Dual LMO attacks, however, the perturbations are
hardly visible. In fact, from Fig. 3 it is noticeable that PGD and AutoPGD attacks apply small perturbations uniformly over the image. While the FW + Dual LMO attack perturbs only small portions of the image, the perturbations are much more visible.


Fig. 2. Adversarial samples on an image with original label 4 (deer).


Fig. 3. Perturbations added to the image with original label 4 (deer).

## 5. Conclusion and Future Work

We compared different attack methods with different metrics. The champion of the comparison is the PGD attack. Although being a very simple attack, it performs very well in terms of misclassification and targeted misclassification rates, is fast, and is almost nondetectable by the human eye in our experiments. AutoPGD, while yielding similar results, is much slower, and hence, comes in second place in our comparison. FW + Dual LMO attack performed very well in terms of duration, misclassification, and targeted misclassification
rates, but the perturbations were much more noticeable. The FGSM attack was the fastest with a high misclassification rate but came last in terms of imperceptibility.

Since we've covered only a small portion of attacks, we plan to extend the attack list by adding more well-known or state-of-the-art methods and extend the experiment domain to black-box attacks as well. Furthermore, we plan to test these attacks on a defended model and compare their performances. Particularly, we are interested to see the difference between AutoPGD and PGD attacks on a defended model.

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<br><br>e-mail: grigor.bezirganyan@tum.de, henrik.sergoyan@tum.de

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# Краткое сравнение между "Белым ящиком", целевыми состязательными атаками противника в глубоких нейронных сетях 

Григор Безирганян и Генрик Сергоян

Технический Университет Мюнхена
e-mail: grigor.bezirganyan@tum.de, henrik.sergoyan@tum.de


#### Abstract

Аннотация Сегодня нейронные сети используются в различных областях, в большинстве из которых важно иметь надежный и правильный вывод. Вот поэтому состязательные атаки делают глубокие нейронные сети менее надежными для использования в областях, где безопасность имеет решающее значение. Следовательно, важно изучить потенциальные методы атаки, чтобы иметь возможность разрабатывать гораздо более надежные сети. В этой статье мы рассматриваем четыре "белых ящика" - целенаправленные состязательные атаки и сравниваем их с точки зрения частоты ошибочных классификаций, частоты целевых ошибочных классификаций, длительности атаки и незаметности. Наша цель - найти атаки, которые были бы эффективны и генерировали бы состязательные выборки с небольшими возмущениями и не обнаруживались бы человеческим глазом.

Ключевые слова: состязательные атаки, надежность, машинное обучение, глубокое обучение.


# ininflueDeveloping Aerial Unmanned Effective Decision Makers 

Sedrak V. Grigoryan and Edward M. Pogossian<br>Institute for Informatics and Automation Problems of NAS RA<br>e-mail: addressforsd@gmail.com, epogossi@aua.am


#### Abstract

Unmanned aerial vehicles (UAVs, drones) and similar unmanned units are becoming more and more involved in various spheres, such as agriculture, emergency situations, battles, etc. however, in decision making there are still a lot they can be improved to avoid human direct involvement in those problems.

To advance in the problem we develop tools to make UAV autonomously effective decision makers, particularly, able to analyze properly given situations and then according to assigned goals select appropriate strategies to achieve the goals.

In the following work we aim to provide a solution for a single UAV which is able to discover units of interest, and select the target to track, manipulate or hit based on expert specified knowledge, as well as discuss further steps.


Keywords: Object, detection, Decision making, Combinatorial problems, Expert knowledge.
Article info: Received 16 August 2022; accepted 26 September 2022.

## 1. Introduction

### 1.1. Problems of Space of UAV Involvements

Involvement of programmatic solutions in various types of UAV-based environments, such as agriculture, emergency situations, battles, and other types of urgent problems, is important and actual problem.

Representation of problems can vary from one to another, while given situation for UAVbased solutions may stay in scope of the following list: maps, emergencies, opponents, their positions, etc.

Overall, it is becoming very important to avoid human involvement in these tasks directly to avoid human causalities, to provide descent support and amount of units involved, thus it is important having decision making modules.

A non-expensive UAV which is able to process the field situation as an image from the top, and make decisions based on the current situation without human involvement is an urgent problem. The advantage of such unit is that it can cost low and has pretty high accuracy and effectiveness.

### 1.2. Programmatic Improvements of UAV Units

Various tasks can be considered in this space, including:
1.2.1. The tasks of adequate processing of situations. The program has to properly capture and parse the current situation based on retrieved data, mostly from images. This is currently not fully solved, however there are some available solutions for certain types of such tasks, e.g. detecting units of interests, such as emergency areas, e.g. fire sources on the images, etc.

Such solutions require:
a. sufficient preliminary inherited knowledge and ongoing data related to the units on the field to be recognized, particularly the ones to identify the own and opponent units, targeting items, tracking objects, etc.
b. proper training and examining the functionality of target models in performing parsing of situations and recognizing there all valuable units (the mistakes might be very costly depending on the problem).
1.2.2. Making valuable decisions in situations UAV can:
a. analyze them to select with respect to (wrt) the goals the most prospective and simultaneously available ones
b. select plans of attaining those targets
c. analyze compositions of actions, strategies for the perspective plans
d. make evaluation of the strategies and perform appropriate strategies to attain the goals.
1.3. To examine our approach, we concentrate on the topic for a battle field strategy games $G$, which provide good way to track situation from the top (similar to UAV images).

We consider this as a problem of certain combinatorial RGT class, where the space of solutions is reproducible game trees [1-8].

RGT problems are specified as follows:

- there are (a) interacting actors (players, competitors, etc.) performing (b) identified types of actions in the (c) specified types of situations;
- there are identified utilities, goals for each actor;
- actions for each actor are defined
- the scope of solutions at the situations are fully determined by them (i.e., are identified as games with perfect information)

Actors perform their actions in specified periods of times and do affect situations by actions in time $t$ by transforming them to new situations in time $t+1$ trying to achieve the best utilities on that situation (goals) by regularities defining these actions.

For example, a way to interpret battle field game G as the RGT problem is:

1. The battling sides can be considered as interacting actors
2. Military units' movements, attacks can be considered as actions
3. The battle field area including military units can be considered as the situations
4. Different situations can be considered as goals: capture objects, destroy enemy units, push frontline.
5. The analysis of given situations are sufficient for selection of proper strategies

### 1.4. Advances of RGT Solvers

1.4.1. There are certain important advances and achievements in cognizers (RGT Solvers) [7] development:

In it was shown that RGT problems are reducible to each other, particularly, to some standard kernel RGT problem K, say, chess, thus, we get an opportunity to integrate the best-known achievements in solving particular RGT problems into RGT Solvers letting us to apply those achievements to any of RGT problem [1].

In RGT solutions, we follow the research lines of Botvinnik, Pitrat, Wilkins and ones successfully started since 1957 in the Institute for Informatics and Automation Problems at the Academy of Sciences of Armenia and based on modeling of expert approaches involving: knowledge bases, knowledge-based algorithms of decision making and matching situations to classifiers, as well as algorithms of revealing and modifying knowledge.

The advances in RGT [1-10] include the following:

1. Solutions for transforming situations for RGT problems, a solution for chess is available. "Generals: Command and Conquer" game is considered as a sample battlefield problem and positive results were achieved for recognition of military units.
2. Knowledge presentation and matching algorithms were developed generally for RGT problems and adequacy was experimented for chess, marketing and other RGT problems.
3. Planning and decision-making algorithms, IGAF and PPIT (including TZT) based on Botvinnik's ideas were developed and tested for network intrusion protection problems and chess problems. Additionally, partial implementation of PPIT algorithms were integrated in general RGT Solver and experimented for chess and other RGT problems.

Various urgent combinatorial problems were investigated as RGT problems including network protection from hacker intrusions [1], single ship defense from various types of attacks $[6,7]$, chess [2, 4], etc.
1.5. We aim to resolve some of above-mentioned tasks by providing programs for UAV, i.e., autonomously effective decision makers, or agents, particularly for type of games $G$ that will allow to process properly situations of G, then according to assigned goals select appropriate strategies for achieving the goals.

In the current work we concentrate on the following problems:
a. From the input images from UAVs detect and classify units of the game G influential for attaining the goals
b. From the input situation including already classified influential units select target to hit.

## 2. Units' detection, classification

Classification of influential units is performed via the recorded images. Popular object detection and image classification methods are now widely based on machine learning solutions, particularly deep convolutional neural networks, e.g. in the following an approach for vehicle detection from aerial images is discussed [11].
In the following we also rely on ML solutions to train a model for influential units' detection and classification.

### 2.1. Creation of Classification Dataset

Based on analysis of available data, we collected influential unit images and videos. From the collected data images were revealed to describe influential units for training the model. We made
a grouping of some classes of influential for game G units into one class, later to be classified as the same. This allows to have much less classes and possibly higher detection rate. The created dataset mostly consists of aerial photos, because UAVs mostly take pictures that way.
We have selected 8 groups of influential for game G classes, then created dataset consisting of their aerial images.

### 2.2. Preparation of Detection Model

Once we have the images as discussed in above section, we prepare it for training models. In the case of the game G unit's detection, the model needs both accuracy and speed, but it is more essential to draw accurate detection conclusions. Some of the studies reveal that YOLO provides better detection and speed combination over other models in various problems, providing real time detection ability [11-16]. Based on the available results we use YOLOv5 as a model to be used for our dataset training and detection.
The trained model gave results of accuracy with the values as follows: detection precision about $80 \%$, recall is close to $60-70 \%$ and mAp about 60. The summary is in Fig. 1.


Fig. 1 Metrics of Training Results.

## 3. Selection of The Target

As described in Introduction chapter we are relying on the achievements of RGT to provide decision making solutions in such problems, particularly the solutions rely on expert knowledge. Here it comes to finding out the knowledge pieces needed in decision making in the game G and specifically for selection a target for UAV managing as we concentrate our attention to that specific game G in the current work.
The experts' analysis and descriptions the following nuclear types [2] of knowledge for game G were revealed.
For the targeting influential units:

1. The class of the $G$ units as classified in section 2, can be reduced to a value in range of $\{1-8\}$ for each class having a specific value.
2. The price of the unit. This is not the actual cost of the unit, but the price of the unit in the battle, describing how much can its damage be. So we assign this a rule of $\{1-8\}$ range depending on the type of target.
3. Other types of expert knowledge also participate in decision making, based on which the decision becomes more accurate.
For own UAV:
4. It also contains specific types of knowledge, in this case this is related to the managing abilities, the decision realization instruments type and power, which determine the target to be resolved.
Based on the following nuclear classifiers we construct classes of units that appear as possible


Fig. 2. The Flow of Target Selection Algorithm.
targets [2, 9]. In the tasks we only consider decisions relevant to the game $G$ by the UAV as our own action. So, the simplified version of goal searching algorithms [2, 10] is applied here. First non-perspective targets are filtered out in the situation. Then by unit price the prioritization is applied and, with some additional corrections the target is selected.
Because the situation is changing, the selected target on each situation can be different.
To increase the confidence of correct selection of the targets, in sequential situations the same logic of target selection is applied several times.
If examined target is confirmed, the confidence is increasing. With attaining certain confidence in certain time period, the target is locked on.
3. Above we discussed the basic approach and some of applied knowledge descriptions for the selection of the targets.
The model of detection of influential units and its metrics were provided in section 2.
Knowledge-based approach adequacy has been discussed in [2, 8, 9].
The performance and the efficiency of programs realizing our UAV approach are attributed as follows:
a. The program is developed in python programming language to provide easy and fast transitions between various experimenting environments.
b. To improve efficiency of the program, when the target is selected, it is only tracked without its recurring detection and matching.
c. Once target is locked on, the program calculates and provides the direction for hitting it.
d. The efficiency of the program is experimented with various video inputs with different frame update rate: frames per second (FPS), resolution, the program provides close to real time results: for HD and FullHD videos with 20-25 fps the program is able to achieve close to real time performance.
e. The prepared program and its performance were tested low power-consuming and GPU enhanced devices, which may be a good fit for UAV setup.

## 4. Future Works

The current solutions demonstrate the positive results of the work, as well as provide background for the future steps.
The next steps of the current works are:

1. The accuracy of the detection of game $G$ units affects the whole flow of target selection and situation processing, decision making, thus improvement of detection is one of essential topics, also due to possible fatal problems in actual application mistakes. For this step we go on the following direction: 1.1. Enhancement of the dataset with new images, 1.2. Enhancement of dataset by machine learning solutions, such as data augmentation, 1.3. Applying machine learning techniques to improve quality of the input 1.4. If the amount of data is sufficient, then classify exact types of units instead of grouping them.
2. Enlarging the scope of considered situation. This assumes enhancing the knowledge for matching situations, which can help in properly selection targets, provide more than one type of actions for involved other than the given single UAV own units, specifying separate targets for own units and the sequence for targets to be hit. The enhancement of knowledge of the experts is an essential part in making decisions and improvement of decision with the increase of expert knowledge is demonstrated in [9], while integration of knowledge-based decision-making algorithms provided in [2,10] also demonstrated their adequacy.
This provides a good background for using the solutions in real UAVs.

## 5. Conclusions

In the following work an approach to describe battle field problem is discussed, where a way to formalize the problem is given. The following results were achieved:

1. From open sources many photo and video data were analyzed, and images were revealed to create a dataset of $G$ units. The dataset consists of 8 classes, each of them containing a group of units functionally equal to the ones defined by experts, to achieve an acceptable accuracy in detection.
2. YOLOv5 model was used for training a model to detect the selected classes, and the results of model performance were demonstrated.
3. By close cooperation with experts of that field certain types of knowledge to properly select the target to be hit were revealed.
4. Algorithms to select the target based on input images, classified objects on that and the knowledge of the field are developed.
5. Experiments were conducted for low power computing units and close to real time processing efficiency is achieved.

Relying on the results achieved in this work and achievements described in the field of RGT problems, we plan the next steps of the work as follows:

1. Collect more data from available sources, enhance the existing dataset by machine learning tools. This allows to achieve better detection and classification accuracy, as well as makes it possible later to more detailed classification instead of grouping them.
2. Enlarge the scope of included problems to consider also agricultural, emergency and other urgent applications, to provide certain types of actions based on decisions it makes using algorithms developed for RGT Solvers [2, 9, 10].
3. Enhance knowledge base for the problems based on expert knowledge to enable various types of actions, including ways of more appropriate target selections, target managing sequence selections, etc.

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<br> e-mail: addressforsd@gmail.com, epogossi@aua.am

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# Разработка программ принятия эффективных беспилотных решений 

Седрак В. Григорян и Эдвард М. Погосян<br>Институт проблем информатики и автоматизации НАН РА<br>e-mail: addressforsd@gmail.com, epogossi@ aua.am


#### Abstract

Аннотация

Беспилотные летательные аппараты (БПЛА, дроны) и подобные беспилотные устройства наряду с возрастающим числом приложений в сельском хозяйстве, управлении при чрезвычайных ситуациях, например боевых и т.д., требуют значительного усовершенствования эффективного принятия решений.

Нами разрабатывается програмы, позволяющие, в частности, анализировать ситуации, а затем в соответствии с поставленными целями выбирать подходящие стратегии для достижения целей.

В работе представлены описание процедуры анализа ситуации для обнаружения целевых обьектов и их отслеживания, анализа версий решений с использованием наличных знаний эксперта, выбора конкретной цели и принятия окончательного решения.

Ключевые слова: обнаружение объектов, принятие решений, комбинаторные задачи, экспертные знания.


# Proof Complexity of Hard-Determinable Balanced Tautologies in Frege Systems 

Anahit A. Chubaryan<br>Yerevan State University<br>e-mail: achubaryan@ysu.am


#### Abstract

Hard-determinable property and balanced property of tautologies are specified as important properties in the study of proof complexities formerly. In this paper harddeterminable and balanced properties are studied together. It is shown that some sequences of hard determinable balanced tautologies have polynomially bounded Frege proofs.


Keywords: Hard-determinable tautologies, Balanced tautologies, Frege systems, Proof complexity characteristics.
Article info: Received 29 June 2022; accepted 29 September 2022.

## 1. Introduction

One of the most fundamental problems in proof complexity theory is to find an efficient proof system for classical propositional logic (CPL). There is a widespread understanding that polynomial time computability is the correct mathematical model of feasible computation. According to the opinion, a truly "effective" system should have a polynomial - size $p(n)$ proof for every tautology of size $n$. In [1] Cook and Reckhow named such a system a supersystem. They showed that $N P=\operatorname{coNP}$ iff there exists a supersystem. It is well known that many systems are not super. This question about the Frege system, the most natural calculi for propositional logic, is still open. In many papers, some specific sets of tautologies are introduced, and it is shown that the question about polynomial bounded sizes for Frege proofs of all tautologies is reduced to an analogous question for a set of specific tautologies. In particular the hard-determinable tautologies and balanced tautologies are introduced in $[2,3]$ as such sets of specific tautologies. In this paper, the hard-determinable and balanced properties are studied together and it is shown that some
sequences of hard-determinable balanced tautologies have polynomial bounded Frege proofs. Using the notions and results of this paper and the results of [3-4] the above-mentioned statement of Cook and Reckhow can be rephrased as follows: $N P=c o N P$ iff in some Frege system of CPL the proofs for all hard-determinable balanced formulas are polynomially bounded.

## 2. Preliminaries

To prove our main result, we recall some notions and notation. We will use the current concepts of the unit Boolean cube ( $E^{n}$ ), a propositional formula, a tautology, a proof system for CPL, and proof complexity. The particular choice of a language for presenting propositional formulas is immaterial in this consideration. However, because of some technical reasons we assume that the language contains propositional variables, denoted by small Latin letters with indices. Logical connectives $\neg, \&, \vee, \supset$, and parentheses (, ). Note that some parentheses can be omitted in generally accepted cases.

### 2.1. Hard-determinable and Balanced Tautologies

Following the usual terminology we call the variables and negated variables literals.
The conjunct $K$ (clause) can be represented simply as a set of literals (no conjunct contains a variable and its negation simultaneously).

In [3] the following notion is introduced.
We call each of the following trivial identities for a propositional formula $\psi$ a replacement-rule:

$$
\begin{gathered}
0 \& \psi=0, \quad \psi \& 0=0, \quad 1 \& \psi=\psi, \psi \& 1=\psi, \psi \& \psi=\psi, \psi \& \neg \psi=0, \neg \psi \& \psi=0, \\
0 \vee \psi=\psi, \psi \vee 0=\psi, 1 \vee \psi=1, \psi \vee 1=1, \psi \vee \psi=\psi, \psi \vee \neg \psi=1, \neg \psi \vee \psi=1, \\
0 \supset \psi=1, \psi \supset 0=\neg \psi, 1 \supset \psi=\psi, \psi \supset 1=1, \psi \supset \psi=1, \psi \supset \neg \psi=\neg \psi, \neg \psi \supset \psi=\psi, \\
\neg 0=1, \neg 1=0, \neg \neg \psi=\psi .
\end{gathered}
$$

Application of a replacement rule to certain word consists in replacing some its subwords, having the form of the left-hand side of one of the above identities by the corresponding right-hand side.
Let $\varphi$ be a propositional formula, let $P=\left\{p_{1}, p_{2}, \ldots, p_{n}\right\}$ be the set of the variables of $\varphi$, and let $P^{\prime}=\left\{p_{i_{1}}, p_{i_{2}}, \ldots, p_{i_{m}}\right\}(1 \leq m \leq n)$ be some subset of $P$.
Definition 1. Given $\sigma=\left\{\sigma_{1}, \sigma_{2}, \ldots, \sigma_{m}\right\} \in E^{m}$, the conjunct $K^{\sigma}=\left\{p_{i_{1}}^{\sigma_{1}}, p_{i_{2}}^{\sigma_{2}}, \ldots, p_{i_{m}}^{\sigma_{m}}\right\}$ is called $\varphi$ determinative if assigning $\sigma_{1}(1 \leq j \leq m)$ to each $p_{i j}$ and successively using replacement rules we obtain the value of $\varphi$ (0 or 1) independently of the values of the remaining variables.

Definition 2. We call the minimal possible number of variables in a $\varphi$-determinative conjunct the determinative size of $\varphi$ and denote it by $d s(\varphi)$.
$\operatorname{By}|\varphi|$ we denote the size of the formula $\varphi$, defined as the number of all logical signs entries in it. It is obvious that the full size of the formula, which is understood to be the number of all symbols is bounded by some linear function in $|\varphi|$.

Definition 3. For sufficiently large $n$ the tautologies $\varphi_{n}$ are called hard-determinable if there is some constant $c$ such that $\log _{\left|\varphi_{n}\right|} d s\left(\varphi_{n}\right) \rightarrow c$ for $n \rightarrow \infty$.
Definition 4. A formula $\varphi$ is balanced if every propositional variable occurring in $\varphi$ occurs exactly twice, once positive and once negative.

Example 1. The tautologies $\varphi_{n}=p_{1} \supset\left(p_{1} \supset\left(p_{2} \supset\left(\neg p_{2} \supset\left(\ldots \supset\left(p_{n} \supset p_{n}\right) \ldots\right)\right)\right)\right.$ are balanced. It is not difficult to see that $d s\left(\varphi_{n}\right)=1$, hence $\varphi_{n}$ are not hard-determinable.

Example 2. The tautologies $Q H Q_{n}=V_{0 \leq i \leq n} \&_{1 \leq j \leq n}\left[V_{1 \leq k \leq i} \bar{q}_{i, j, k} \vee V_{i<k \leq n} q_{k, j, i+1}\right](n \geq 1)$, are balanced. Put $Q_{i, j}=V_{1 \leq k \leq i} \bar{q}_{i, j, k} \vee V_{i<k \leq n} q_{k, j, i+1}(n \geq 1,0 \leq i \leq n, 1 \leq j \leq n)$, then $Q H Q_{n}=$ $V_{0 \leq i \leq n}\left(Q_{i 1} \& Q_{i 2} \& \ldots \& Q_{i j} \& \ldots \& Q_{i(n-1)} \& Q_{i n}\right)$ and therefore $d s\left(Q H Q_{n}\right)$. It is not difficult to see, that $\left.\left|Q H Q_{n}\right|=\frac{3 n^{2}(n+1)}{2}-1 \right\rvert\,$, hence $Q H Q_{n}$ are hard-determinable as well.

### 2.2. Proof Systems and Proof Complexities

Let us recall some notions from [1].
A Frege system $\mathcal{F}$ uses a denumerable set of propositional variables, a finite, complete set of propositional connectives; $\mathcal{F}$ has a finite set of inference rules defined by a figure of the form $\frac{A_{1} A_{2} \ldots A_{m}}{B}$ (the rules of inference with zero hypotheses are the schemes of axioms); $\mathcal{F}$ must be sound and complete, i.e. for each rule of inference $\frac{A_{1} A_{2} \ldots A_{m}}{B}$ every truth-value assignment, satisfying $A_{1} A_{2} \ldots A_{m}$, also satisfies $B$, and $\mathcal{F}$ must prove every tautology.

In the theory of proof complexity two main characteristics of the proof are: $l-$ complexity to be the size of a proof ( $=$ the sum of all formulae sizes) and $t$-complexity to be its length (= the total number of lines). The minimal $l$-complexity ( $t$-complexity) of a formula $\varphi$ in a proof system $\Phi$ we denote by $l_{\varphi}^{\Phi}\left(t_{\varphi}^{\Phi}\right)$.

The polynomial equivalence ( $p-l$--equivalence, $p-t$--equivalence) of two proof systems by some proof complexity measure means that the transformation of any proof in one system into a proof in another system can be performed with no more than polynomial increase of proof complexity measure.

It is well known that any two Frege systems are $p-l$-equivalent ( $p-t$-equivalent).
Let $M$ be some set of tautologies.
Definition 5. We call the $\Phi$-proofs of tautologies from the set $M t$-polynomially ( $l$ - polynomially) bounded if there is a polynomial $p()$ such that $t_{\varphi}^{\phi} \leq p(|\varphi|)\left(l_{\varphi}^{\phi} \leq p(|\varphi|)\right)$ for all $\varphi$ from $M$.

### 2.3. Former Results

It was previously proven that
a) tautologies without hard-determinability condition have $t$-polynomially ( $l$ - polynomially) bounded proofs in all systems of CPL [4],
b) hard-determinability condition is sufficient (but not necessary) to obtain exponential lower bounds for both proof complexities of tautologies in"weak" proof systems of CPL (Cutfree sequent, Resolution, Cutting planes etc.) [4],
c) hard-determinability condition is not sufficient for exponential lower bounds of proof complexities in Frege systems: for some examples of hard-determinable formulas the $t$ polynomially ( $l$ - polynomially) bounded Frege-proofs are given in [2].
Some proof systems of CPL (calculus of structures with deep inference rules), where the author considers only formulas in negation normal form, are studied in [3], where among the rest of the results it is proved that
a) the set of above mentioned balanced formulas $Q H Q_{n}$ have polynomially bounded proofs in one of the studied system $s K S$,
b) the relations between the proof complexities in the system $s K S$ and the Frege systems are unknown for the present.

## 3. Main Result

Let $F$ be some Frege system with inference rule modus ponens.
Theorem 1. The $F$-proofs of tautologies $Q H Q_{n}(n \geq 1)$ are $t$-polynomially (t-polynomially) bounded.

To prove, we use the method of [2] for description of some polynomially bounded proof of $Q H Q_{n}$ direct in $F$ by reducing it to $F$-proofs of well-known tautologies

$$
\text { PHP } P_{n}=\&_{0 \leq i \leq n} V_{1 \leq j \leq n} p_{i j} \supset V_{0 \leq i<k \leq n} V_{1 \leq j \leq n}\left(p_{i j} \& p_{k j}\right)(n \geq 1)
$$

presenting the Pigeonhole Principle. It is proved in [5] that the set of these formulas is $t$ polynomially (l- polynomially) bounded.

The following two auxiliary statements will be of use:
Lemma 1. Given arbitrary formulas $\alpha, \beta, \gamma, \alpha_{i}, \beta_{i}, \alpha_{i j}$ and $\beta_{i j}$, the $F$-proofs of the following tautologies are t-polynomially (l-polynomially) bounded:

1) $\alpha \vee \alpha^{-}$,
2) $(\alpha \supset \beta) \supset((\beta \supset \gamma) \supset(\alpha \supset \gamma))$,
3) $\left(\beta^{-} \supset \alpha\right) \supset(\alpha \supset \beta)$,
4) $\alpha_{1} \supset\left(\alpha_{2} \supset\left(\ldots \supset\left(\alpha_{k} \supset \alpha_{1} \& \alpha_{2} \& \cdots \& \alpha_{k}\right) \ldots\right)\right)(k \geq 2)$,
5) $\alpha \vee \alpha^{-} \supset \beta_{1} \vee \cdots \vee \beta k \vee \alpha \vee \beta k+1 \vee \cdots \vee \beta k+r \vee \alpha^{-} \vee \beta k+r+1 \vee \cdots \vee \beta k+r+t$
$(k \geq 1, r \geq 1, t \geq 1)$,
6) $\neg\left(V_{1 \leq i \leq k} \&_{1 \leq j \leq m} \alpha_{i j}\right) \supset \&_{1 \leq i \leq k} V_{1 \leq j \leq m} \bar{\alpha}_{i j}(k \geq 1, m \geq 1)$
7) $\&_{1 \leq i \leq k}\left(\beta_{1 i} \vee \beta_{2 i}\right) \supset \neg\left(V_{1 \leq i \leq k}\left(\bar{\beta}_{1 i} \& \bar{\beta}_{2 i}\right)\right)(k \geq 1)$.

The proof is obvious.
Lemma 2. Let $Q_{i j}$ and $Q_{k j}(0 \leq i<k \leq n, 1 \leq j \leq n)$ be the above denoted subformulas of $Q H Q_{n}$, then $F$-proofs of the formulas $Q_{i j} \vee Q_{k j}$ be t-polynomially (l-polynomially) bounded.

The proof follows from the fact of existence of some $s$ and $m$ ( $1 \leq s \leq n, 1 \leq m \leq n$ ) such that $Q_{i j}$ contains $q_{s j m}$ and $Q_{k j}$ contains $\neg q_{s j m}$, and also from 1) and 5) of Lemma 1.
From 6) of Lemma 1 we infer for the formula $Q_{n}=V_{0 \leq i \leq n} \&_{1 \leq j \leq n} Q_{i j}$.
Condition 1. The F-proofs of the formulas

$$
\neg Q H Q_{n} \supset \&_{0 \leq i \leq n} V_{1 \leq j \leq n} \neg Q_{i j}
$$

are $t$-polynomially (l-polynomially) bounded.
Put

$$
\begin{equation*}
\text { PHP }{ }_{n}^{\prime}=\&_{0 \leq i \leq n} V_{1 \leq j \leq n} \neg Q_{i j} \supset V_{0 \leq i<k \leq n} V_{1 \leq j \leq n} \neg\left(Q_{i j} \& \neg Q_{k j}\right) \tag{1}
\end{equation*}
$$

The formulas (1) are obtained from the $P H P_{n}$ by the corresponding substitutions. Hence,
Condition 2. The F-proofs of the formulas (1) are t-polynomially (l-polynomially) bounded.
Let

$$
A_{n}=V_{0 \leq i<k \leq n} V_{1 \leq j \leq n}\left(\neg Q_{i j} \& \neg Q_{k j}\right) .
$$

Using conditions (1), (2), and item 2) of Lemma 1, we obtain
Condition 3. The $F$-proofs of the formulas $\neg Q H Q_{n} \supset A_{n}$ are $t$-polynomially (l-polynomially) bounded.

From Lemma 2 and item 4) of Lemma 1 we have
Condition 4. The F-proofs of the formulas

$$
B_{n}=\&_{0 \leq i<k \leq n} \&_{1 \leq j \leq n}\left(Q_{i j} \vee Q_{k j}\right)
$$

are $t$-polynomially (l-polynomially) bounded, and from item 7) of Lemma 1 it follows that the $F$ proofs of the formulas $\neg A_{n, m}$ are $t$-polynomially ( $l$-polynomially) bounded as well.

From the conditions (3), (4), and item 3) of Lemma 1 we have a $t$-polynomial (l-polynomial) bound for the $F$-proofs of $Q_{n}$.

Corollary1. There are hard-determinable balanced formulas the $F$-proofs of which are $t$ polynomially (l-polynomially) bounded.

## 4. Conclusion

Using the polynomial equivalence of different Frege systems [1], the above mentioned result of Cook and Reckhow can be rephrased as follows: $N P=c o N P$ iff in some Frege system of CPL the proofs for all hard-determinable balanced formulas are polynomially bounded.

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# Сложности выводов трудно-определяемых балансированных формул в системах Фреге 

Аанаит А. Чубарян<br>Ереванский государственный университет<br>e-mail: achubaryan@ysu.am


#### Abstract

Аннотация

Ранее свойство трудно-определяемости и свойство балансированности тавтологий были выдлены как важные свойства в исследованиях сложностей выводов. В настоящей статье свойства трудно-определяемости и балансированности изучаются совместно. Доказана полиномиальная ограниченность выводов в системах Фреге для некоторого класса трудно-определяемых балансированных формул. Ключевые слова: трудно-определяемые тавтологии, балансированные тавтологии, системы Фреге, характеристики сложностей выводов.


# Research of Obfuscated Malware with a Capsule Neural Network 

Timur V. Jamgharyan<br>National Polytechnic University of Armenia<br>e-mail: t.jamgharyan@yandex.ru


#### Abstract

The paper presents the results of a research of using transfer training of the capsule neural network to detect malware. The research was carried out on the basis of the source code of malware using the context-triggered piecewise hashing method. The source codes of malware were obtained from public sources of software. Verification of the capsule neural network learning results was carried out using a trained convolutional neural network, and publicly available sources of test to malware. The research was conducted on six types of malware. Software source code, part of capsule neural network training datasets, pre-trained capsule neural network, and full research are publicly available at https://github.com/T-JN


Keywords: Capsule neural network, Context triggered piecewise hashing, Edit distance, Intrusion detection system, Transfer learning.
Article info: Received 9 June 2022; accepted 24 November 2022.

## 1. Introduction

Malware injected into Infrastructure through zero-day vulnerabilities in network equipment is a huge cybersecurity problem. The network infrastructure (NI) protection architecture implies the construction of a multi-level, complementary security system. Part of the NI security design is an intrusion detection system (IDS).
In the studies [1]-[5], the types of IDS, the ways of their application and the mechanisms of their work are considered in detail. «Classic» IDS can be classified as:

* host-based IDS, that is detection of attacks on a specific network node,
* network-based IDS, that is, detecting attacks on the network or its segment.

Existing IDS that do not use machine learning (ML) in their functionality (both proprietary and open source) [6]-[9], have one common drawback: they all respond to the threat that is embedded in the rule sets. There is also a high probability of various false positives: (true positive, true negative, false positive, false negative) [10]. Malware is the most common threat
vector in most operating environments [11]. The IDS software ecosystem offers many utilities and application suites that can help collect signals from all types of network traffic [12].
For IDS operating without the use of ML at different levels of the Open System Interconnection (OSI) model [13], the task of detecting malware modifications was secondary. Basically, the task of detecting and neutralizing malware was assigned to antivirus software. But with the convergence of attacks at different levels of the OSI model and the emergence of softwaredefined networks (SDN), new types of threats and possible attacks arise, the neutralization of which by «standard» methods is difficult [14]-[15]. New systematic approaches are required to solve these problems. With the increase in the growth of attacks built on the basis of ML and machine-to-machine (M2M), new threats to the NI also arise. The requirements for security systems are increasing. The convergence of system, network and cloud services increases both the «attack surface» [16] and the «attack space power» [17]. Of particular danger are attacks «designed» using ML [18]-[20]. Researchers are working on the application of ML to create and build a new type of IDS [21-25]. Unlike «classic» IDS, built on the basis of ML can be further trained, being in one way or another a malware generator [26]-[28]. At this stage, both conceptually new solutions in the field of ML application in IDS are being developed, as well as improvements to existing ones. The papers [29]-[32] consider the issues of using ML to create one or another type of IDS. Researchers and developers of ML-based IDS are faced with a large number of tasks that need to be solved, due to the novelty of this area of information security.

- The task of having annotated data for training a neural network (Annotation is the process of labeling raw data so that it can become training for machine learning [11]). No algorithm can handle really bad data. There are many different requirements for training datasets, in particular, representativeness and «noiselessness». [33]. Unlike neural networks that process images, sound, text, etc., for which there are verified datasets [34][39], datasets for training an IDS must to some extent, consist of malware. Researchers have access to certain resources that supply research malware [40]-[46], but these resources make them public with a delay.
- The task of increasing the learning rate of IDS built on the basis of ML. Unlike other neural networks where the main attention is paid to the quantity and quality of training data, in intrusion detection systems built on the basis of ML, in many cases, the speed of learning is also important. As shown in [47], since the emerging malware not included in any database has a different data distribution compared to the original training samples, the efficiency of model detection will decrease when it encounters new malware.
- The task of correctly calculating the degree of threat in an attack using ML [48]. When developing an IDS based on ML, it is necessary to correctly calculate the degree of threat to the protected NI.
In addition to general tasks, there are also specific tasks: since each group and type of malware requires its own specific detection methods [49]-[50].
- Detection based on signature analysis, where a database of malware hashes is used as a signature,
- Detection based on Indicator of Compromise (IoC). It is a set of artifacts based on which malware can be detected: registry branches, loadable libraries, IP addresses, byte sequences, software versions, date and time triggers, ports involved [51].
- Research based on context triggered piecewise hashing (CTPH), (context triggered piecewise hashing is a method of calculating piecewise hashes from input data [52]). Malware developers use various techniques to change the original malware signature to make hashes harder to detect: encryption, obfuscation, reordering of files and libraries, re-distribution and code building in order to fool the detection system, giving malware a
new look and changing the hash values. In this case, malware remains undetected for some time [53].
Various researchers are considering the use of CTPH techniques for malware detection. In [54], the issue of applying transfer learning to solve the problem of malware domain bias is considered, and in [55], the issue of automatic malware family identification and classification through online clustering is considered. But the main issues of preparing malware datasets and training IDS based on ML remain open. The issue of increasing the performance of an IDS based on ML with a small set of training datasets remains relevant. In this paper, a method for applying transfer learning of a capsule neural network with the calculation of CTPH and editing distance to increase the learning rate and detection of malware is investigated. The Levenshtein method [56] (Equation 1) and the method using the ssdeep program [57] were chosen as the mathematical apparatus for calculating the editorial distance. To assess the quality of binary learning, the Matthews correlation (Equation 2) [58] was used. The source codes of the malware for creating a set of annotated datasets were taken from open sources. The following malware was used: mimikatz, athena, engrat, grum, surtr, dyre.

$$
D(i, j)=\left\{\begin{array}{lr}
0, & i=0, j=0  \tag{1}\\
i, & j=0, i>0 \\
j, & i=0, j>0 \\
\min \{ & \begin{array}{rl}
D(i, j-1)+1, j>0, i>0
\end{array} \\
& \begin{array}{ll}
D(i-1, j)+1+m(M[i], N[j]),
\end{array}
\end{array}\right.
$$

Levenshtein editorial distance calculation equation,
where, $D$ - the editorial distance, $M, N$ - the length of strings obtained as a result of CTPH over some alphabet (in this case HEX), $i$ - remove step from the first line, $j$-insert into the first line.

$$
\begin{equation*}
\phi=\frac{T P \times T N-F P \times F N}{\sqrt{(T P+F P)(T P+F N)(T N+F P)(T N+F N)}}, \tag{2}
\end{equation*}
$$

where,
$\phi$ - Matthews correlation
$T P$ - true positive,
$T N$-true negative,
$F P$-false positive,
$F N$ - false negative.
A capsule neural network was chosen as a transfer learning model. The choice of the capsule network is due to the following reasons:

- the capsule network does not require a large amount of training data, which is critical for this research,
- the capsule network explores hierarchical relationships, which allows detecting possibly probable versions, in the presence of a primary code (a fragment of the main code) of malware,
- the capsule network allows searching even in obfuscated source code with a minimum malware representativeness value,
- the capsule network is the most easily adaptable to changing the learning algorithm compared to other neural networks.


## 2. Diagrams of Neural Networks



Fig.1. Diagram of a capsule neural network.

## - Different memory cell

Probablistic capsule hidden cell
-
Output cell
$\longrightarrow$ Entry node
The nonlinearity function of the capsule network is determined by (Equation 3) [59].

$$
\begin{equation*}
\boldsymbol{v}_{\boldsymbol{i}}=\frac{\left\|s_{i}\right\|^{2}}{1+\left\|s_{i}\right\|^{2}} \frac{s_{i}}{\left\|s_{i}\right\|}, \tag{3}
\end{equation*}
$$

where, $s_{j}$ - the result obtained in the previous step, $\boldsymbol{v}_{\boldsymbol{i}}$ - the result obtained after applying the nonlinearity. The left side of the equation performs additional compression, and the right side of the equation performs unity scaling of the output vector.

The trained convolutional neural network (Fig. 2) was chosen as a test to check the reliability of the output data. As «weight coefficients» of the convolutional neural network, the value of CTPH was calculated the used ssdeep software.


Fig. 2. Diagram of a convolutional neural network.


Verification of the results obtained from both neural networks was carried out using public malware detection services [60]-[61]. The developed software algorithm is shown in Fig.3.


Fig. 3. Algorithm of the developed software.

## Algorithm operation:

Operations on the input data of the research.

- The dataset generated from the malware source code was obfuscated using various tools [62][63] and prepared for training a capsule neural network (dataset 1).
- The same non-obfuscated dataset (dataset 2) generated from the malware source code was prepared to train a convolutional neural network.
A total of 1000 annotated datasets of various sizes (20.40, 80, 128, 256, 512, 1024 bytes) were prepared for mimikatz, athena, engrat, grum, surtr, dyre software.
Steps 1, 2: input of the initial malware dataset into the trained neural networks and the conversion module,

Step 3: converting the source dataset to javascript object notation (JSON) format and setting the CTPH step size,

Step 4: calculation of the edit distance by the Levenshtein method,
Step 5: computation CTPH using ssdeep software,
Step 6: comparison of the values calculated by the Levenshtein method and using the ssdeep software,

Step 7:filtering the training datasets of neural networks from «noise» (the full implementation of this part of the algorithm is presented in [33]),

Step 8: training capsular neural network,
Step 9 training convolutional neural network,
Step 10 compute the Matthews correlation and resize the training datasets.
$>\phi=-1$ the received output data of both neural networks go beyond the value tolerance
$>\phi=1$ the resulting outputs of both neural networks are correct (within the permissible deviation value)
$>\phi=0$ the resulting output of both neural networks is random
Steps 11, 12: reconfiguring the training datasets and resizinge the CTPH.
Table 1 presents the results of calculating the value of CTPH and the editorial distance between the hashes of the obfuscated source code of mimikatz software using capsular, convolutional neural networks, as well as ssdeep software.

Table 2 shows the results of calculating the value of the context-piecewise hash of the obfuscated compiled source code and the editorial distance between the hashes of the mimikatz software using capsular, convolutional neural networks, and also the ssdeep software.

In the research, datasets used a comparison between files 20-40, 20-80, 20-128, 20-256, 20512, 20-1024 bytes, as well as combinations of 40-512, 40-1024, 128-512, $128-1024$ bytes for mimikatz, athena, engrat, grum, surtr, dyre malware.

## 3. Results

Table 1.The results of computing the value of CTPH and the editorial distance between the hashes of the obfuscated source code of mimikatz software

|  | mimikatz file hash values (20 byte) | mimikatz file hash values (512 byte) |  |  | Percentage of <br> malware <br> samples <br> computed using <br> convolutional <br> neural <br> networks |  |  | Percentage of malware samples computed using capsule neural network |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  | Training epoch |  |  | Training epoch |  |  |
|  |  |  |  |  | I | II | III | I | II | III |
| 1. | $\begin{array}{r} \text { b9be58b87140f922969c } \\ 905236829 \mathrm{~d} 2436 \mathrm{c} 34400 \end{array}$ | ef73afe0b3862206e112 400dc97a6920c1240ca2 | 36 | 10 | 4 | 2 | 9 | 8 | 19 | 39 |
| 2. | e1077e747c9486dce1bf da820c078fe300a901fb | 081cdfaf631a003a5a5d fa678b52af5c0eb2cbd3 | 36 | 13 | 6 | 8 | 7 | 16 | 27 | 42 |
| 3. | $\begin{aligned} & \hline \text { d86c9ca3861e333dc337 } \\ & \text { 6fc5565943551389edd6 } \end{aligned}$ | $\begin{aligned} & \text { 72840526d3cecbba084e } \\ & \text { ef91aed9c52cd94855d5 } \end{aligned}$ | 35 | 25 | 18 | 9 | 9 | 24 | 52 | 78 |
| 4. | bd72fda18edc004d5181 <br> b57e48a757ac2ed94444 | $\begin{aligned} & \text { 783e9520a25faca4f815 } \\ & \text { 2dfc092d7d67e359c5f6 } \end{aligned}$ | 35 | 28 | 21 | 22 | 24 | 8 | 10 | 12 |
| 5. | 8ab1d3267a46f953c73b 4154b1a261a8e02493d8 | $\begin{aligned} & \text { ad523321e582956d7b51 } \\ & \text { e9f4bc3763d9305231dc } \end{aligned}$ | 30 | 11 | 3 | 7 | 3 | 34 | 54 | 82 |
| 6. | dc990c540fc50debf0cd c178101ab107acaef9fe | f2ba969ed8f8ecc7ce57 c54c39de5333cf0d6a8e | 36 | 23 | 11 | 16 | 21 | 16 | 28 | 65 |
| 7. | b137df3d2083c226f985 c0494a9cef753034ac6d | f7fd9ed34bc6ead485bd 5e7c1b9f9f13f30fddba | 34 | 13 | 10 | 9 | 12 | 16 | 27 | 46 |
| 8. | 9efa06fa6567be9554db 5c351da39c9c084306e0 | f7fd9ed34bc6ead485bd 5e7c1b9f9f13f30fddba | 33 | 21 | 15 | 15 | 17 | 31 | 46 | 79 |
| 9. | $\begin{aligned} & \text { 4f5ec65628d2bde662a4 } \\ & 08854 \mathrm{a} 41 \mathrm{caea} 98 \mathrm{c} 0 \mathrm{f} 44 \mathrm{f} \end{aligned}$ | $\begin{aligned} & \text { f5cd09b85a44df103b21 } \\ & \text { ea9c4d02c564fcb19191 } \end{aligned}$ | 35 | 64 | 32 | 30 | 42 | 38 | 37 | 48 |
| 10. | $\begin{aligned} & \text { 5329b04a348368967844 } \\ & \text { f421453563001ad4ab89 } \end{aligned}$ | 37a56e3a4acbef542099 | 36 | 22 | 8 | 11 | 16 | 27 | 48 | 61 |
| 11. | 95a56dfdfd7c8550afb8 ab2474916bb63e58bb15 | 37a56e3a4acbef542099 4c0d7864125e53f5aaa3 | 33 | 16 | 12 | 13 | 15 | 27 | 41 | 68 |
| 12. | $\begin{gathered} \text { aececb9dccd29fd5dd9 } \\ \text { c0559ad62afb84af374b2 } \end{gathered}$ | 51168e0c2ab45361cf05 834a721cd4aba48098be | 34 | 19 | 11 | 12 | 18 | 36 | 49 | 73 |
| 13. | 14791ec8ec19ca534367 <br> c54f008b8439eea89f09 | 497a16d6dd757f05fb88 4994c71bea880e87ad18 | 35 | 11 | 18 | 29 | 25 | 37 | 49 | 68 |
| 14. | dbfb0b8c0a28ea8bade 6306f9e8589ee1c310a39 | c6ca0e98e0a66c45838f b254aec474553850ab91 | 34 | 16 | 14 | 21 | 29 | 52 | 58 | 71 |
| 15. | $\begin{aligned} & \text { c91e176518b7e42450e2 } \\ & \text { c28d45bf31a1b3178240 } \end{aligned}$ | 7ad0cc0f4ba8c767fac7 f0a4f7ec192b3a60ec9e | 36 | 18 | 16 | 19 | 28 | 29 | 43 | 68 |
| 16. | 04b66940a08ac7adb0cd f19382a8169d0c256c09 | 5db88a72cdcfe90ff987 <br> 1eae5bf8d2b617d73b0a | 37 | 26 | 11 | 19 | 36 | 39 | 56 | 73 |
| 17. | $\begin{aligned} & \text { 67b4a269a360b994d776 } \\ & 9 \mathrm{e} 4 \mathrm{~b} 40220 \mathrm{c} 8 \mathrm{~b} 59 \mathrm{c} 219 \mathrm{~b} 0 \end{aligned}$ | $\begin{aligned} & \text { fa926a049a1d9d72126b } \\ & \text { d07f1a1b87326b5e355b } \end{aligned}$ | 34 | 41 | 27 | 11 | 29 | 26 | 58 | 61 |
| 18. | c2cdacd22e871ecef12b 0cbc8caf4559eecfa084 | 817c64fed50532e58dd2 1a8812c65fe10a250bd0 | 36 | 16 | 15 | 16 | 26 | 31 | 46 | 74 |
| 19. | $\begin{aligned} & \text { 4202fc70b1301ec50b1f } \\ & \text { 64ca525de6d31825787d } \end{aligned}$ | 38bc177d79492834356f 1cce4f9120599f41e952 | 36 | 18 | 17 | 19 | 21 | 28 | 37 | 49 |
| 20. | $\begin{gathered} \text { 20b5c47533cb97d72f9 } \\ \text { 0895ea1ffe27695063e54 } \end{gathered}$ | $\begin{aligned} & \text { 818b59add29456248836 } \\ & 864 d 46 \mathrm{c} 146 \mathrm{~d} 9 \mathrm{~d} 930 \mathrm{~d} 8 \mathrm{a} 2 \end{aligned}$ | 37 | 19 | 8 | 16 | 34 | 24 | 37 | 58 |

In training epochs 1-3, the results of the capsular neural network are better than the results of the convolutional neural network and ssdeep software, except for file №4 in the dataset, which is included in the statistical error.

Table 2. The results of calculating the value of CTPH and editorial distance between hashes of the compiled mimikatz source code.

|  | mimikatz file hash values (20 byte) | mimikatz file hash values (512 byte) |  |  | Percentage ofmalware samplescomputed usingconvolutionalneuralnetworksTraining epoch |  |  | Percentage of malware samples computed using capsular neural network |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  | Training epoch |  |  |
|  |  |  |  |  | I | II | III | I | II | III |
| 1. | d7e4e9abedd0949b8bcf f30c7abbdad97b182be8 | $\begin{gathered} \text { 51f028f6b078f51583e0 } \\ \text { a048d9bc577b6a4e17b9 } \end{gathered}$ | 37 | 25 | 23 | 31 | 42 | 17 | 19 | 23 |
| 2. | 2c0e9d614fab60e18bd4 2e99659974a3d298a9ae | 7f966e5a707dd69c13b5 de45c9765a9be437e642 | 35 | 16 | 18 | 14 | 22 | 8 | 11 | 9 |
| 3. | f76606cb6fae082991eb 271af5ab7629d592cb04 | $\begin{aligned} & \text { fb96549631c835eb239c } \\ & \text { d614cc6b5cb7d295121a } \end{aligned}$ | 32 | 28 | 27 | 36 | 45 | 16 | 17 | 14 |
| 4. | 14da593832768f0a08e8 ecd46363936eef096dcc | 72ac7a00a3c2a0a825cd 016d71b0d587c6cc3f46 | 36 | 23 | 16 | 22 | 34 | 18 | 20 | 16 |
| 5. | 7f01a23afa1bcecdfdbb 25b953c4f15366eaba51 | $\begin{aligned} & \text { 35139ef894b28b73bea0 } \\ & 22755166 \mathrm{a} 23933 \mathrm{c} 7 \mathrm{~d} 9 \mathrm{cb} \end{aligned}$ | 37 | 37 | 34 | 41 | 48 | 27 | 29 | 23 |
| 6. | 1ca12a53c82cdd508054 bdcdbe5256ccdd44c13c | 918b1c05e576f4b90fce <br> 15a06bc3442d72852a3c | 35 | 48 | 44 | 53 | 61 | 34 | 31 | 28 |
| 7. | a7f0499bf3eb6180d4da 748426822404 e 46 dea 13 | $\begin{aligned} & \text { 4759f2ba1ba20f493664 } \\ & \text { dbf5e36c 1a1ec0d75658 } \end{aligned}$ | 36 | 15 | 11 | 13 | 12 | 8 | 2 | 3 |
| 8. | $\begin{aligned} & \text { aec2a4accb7ca456a57a } \\ & \text { c4426e8f51c2e6a8b143 } \end{aligned}$ | $\begin{aligned} & \text { 902a2d132f213700b5de } \\ & \text { fbefe7567f68ca8e234a } \end{aligned}$ | 35 | 19 | 18 | 26 | 29 | 16 | 10 | 13 |
| 9. | $\begin{gathered} \text { 582d2ceff8f4f493f3a9 } \\ \text { d45c71286255946a7d37 } \end{gathered}$ | b2fd9a1405ba74fc360e 1784961176b2b88bf5c9 | 37 | 39 | 28 | 48 | 57 | 25 | 23 | 12 |
| 10. | $\begin{aligned} & \text { a25a87930b155282e138 } \\ & \text { 35142ad63cea1994d02d } \end{aligned}$ | $\begin{aligned} & \mathrm{c} 47419 \mathrm{fdd} 4 \mathrm{~d} 6 \mathrm{f} 146 \mathrm{e} 430 \\ & \text { 64b9ddb859a250404500 } \end{aligned}$ | 36 | 53 | 47 | 40 | 57 | 34 | 29 | 47 |
| 11. | 2f7b14912dddcf7c1c7a ebb49955cb5bf0ab3257 | $\begin{aligned} & \text { b521d7652866027a7e5b } \\ & \text { 43c6269d7c81ffb5a86e } \end{aligned}$ | 36 | 28 | 30 | 37 | 44 | 14 | 19 | 23 |
| 12. | $\begin{gathered} \text { fd5fd2f7953cf5630f74 } \\ \text { c2933b378d4381367ddd } \end{gathered}$ | 9de4bfa1fdb6c90637d3 5492ec14ee10a3967997 | 33 | 56 | 49 | 53 | 67 | 42 | 48 | 34 |
| 13. | e88dac72cd8ac64360d9 <br> 5fb15e8ea9aaa8794f8c | 1eb796fd1ff7dda036fc a37d0f31aab19dedab1a | 37 | 24 | 29 | 48 | 52 | 17 | 23 | 15 |
| 14. | $\begin{aligned} & \hline \text { efa91cc773ee2c32ba51 } \\ & \text { 2ffce8db8a3760bda564 } \end{aligned}$ | $\begin{aligned} & \text { 99828f68be57c53ff954 } \\ & \text { 5f79e32bdb36050bf93b } \end{aligned}$ | 32 | 19 | 27 | 29 | 37 | 13 | 18 | 28 |
| 15. | f9980d6122acf1bf54a6 8e49d15507fbc3ce7c1f | $\begin{gathered} \text { 2400b40333821b00b5d0 } \\ \text { b67f20f5f0e30ebf02dd } \end{gathered}$ | 36 | 56 | 44 | 58 | 63 | 37 | 34 | 39 |
| 16. | $\begin{aligned} & \text { c5d4d95ce32029e1150a } \\ & \text { 20d2f836b7b2c6e49546 } \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline \text { dfb380d8b0709104c606 } \\ & 978092 \mathrm{c} 7164160 \mathrm{f} 32887 \end{aligned}$ | 37 | 29 | 27 | 35 | 38 | 21 | 17 | 34 |
| 17. | 5156507d0b07bd9eaafe 56815e1a04a0eaa1a8e9 | bd951f174a8f0f211c62 bc1869d69f581788ee59 | 37 | 48 | 27 | 44 | 56 | 25 | 38 | 14 |
| 18. | 14fd3fa5756432336c73 656c76f4751aa6f707f9 | b9acd4446a9ee133799f a3d8f3e35e001c616776 | 37 | 16 | 24 | 36 | 38 | 8 | 10 | 11 |
| 19. | f1d8238c9141f46246bf 2193908b1be6f87b09f8 | f1513655d577bf56bcf86 2b1851e66bb683d373c | 33 | 56 | 48 | 56 | 61 | 32 | 27 | 46 |
| 20. | 50effcaad368f00bfc71 2105a708ff917f9f95d0 | $\begin{aligned} & \text { 49a48ed249c7b82959aa } \\ & \text { 85b9470938bbcc9c45cc } \end{aligned}$ | 36 | 36 | 27 | 38 | 46 | 16 | 28 | 31 |

In epochs 1-3 of training for compiled software, the results of the capsule neural network are worse worse than the results of the convolutional neural network and ssdeep software.


Fig. 4. CTPH results of the obfuscated mimikatz source code.


Fig. 5. CTPH results of obfuscated and compiled mimikatz source code.

The use of a convolutional neural network is not always justified, since the degree of detection is comparable to the degree of detection by ssdeep software. The use of a capsule neural network for malware detection is justified in the presence of the source code (even in an obfuscated state), since even after the first training epoch, the detection results are not worse (and in most cases better) than the detection results using ssdeep and a trained convolutional neural network.
Tables 3 and 4 present the results of the studies of the operation of capsule and convolutional neural networks, based on datasets obtained from the obfuscated mimikatz source code with three training epochs and a variable block size of CTPH.

Table 3. Number of detected threats.

|  | $\begin{aligned} & \text { Number of datasets } \\ & \text { (dataset 2) } \end{aligned}$ | The number of samples detected and classified as threats on different sizes ( $20,40,128$ bytes) and three epochs (I, II, III) of training by a capsule neural network |  |  |  |  |  |  |  |  | The number of samples detected and classified as a threat at different sizes ( $20,40,128$ bytes) and three epochs (I, II, III) of training by a convolutional neural network |  |  |  |  |  |  |  |  | Number of detected but mismatched malware samples * |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{array}{r} \text { CTPN } \\ \text { (byt } \end{array}$ |  | 20 |  |  | 40 |  |  | 128 |  |  |  | 20 |  |  | 40 |  |  | 128 |  |  |  |  |
| $\begin{array}{r} \text { Train } \\ \text { epo } \\ \hline \end{array}$ | $\begin{aligned} & \text { ning } \\ & \text { och } \end{aligned}$ | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III |
| 100 | 100 | 7 | 7 | 9 | 11 | 13 | 12 | 12 | 15 | 18 | 3 | 3 | 4 | 4 | 6 | 6 | 9 | 10 | 1 | - | - | 1 |
| 200 | 200 | 10 | 11 | 11 | 12 | 14 | 16 | 17 | 17 | 21 | 5 | 4 | 6 | 6 | 8 | 5 | 8 | 5 | 6 | - | 1 | 2 |
| 300 | 300 | 12 | 12 | 14 | 16 | 18 | 23 | 28 | 29 | 22 | 8 | 7 | 8 | 8 | 9 | 11 | 13 | 15 | 16 | 1 | 1 | 2 |
| 350 | 350 | 12 | 13 | 15 | 15 | 16 | 18 | 21 | 26 | 25 | 7 | 7 | 11 | 10 | 12 | 18 | 16 | 18 | 19 | 2 | 2 | 3 |
| 450 | 450 | 14 | 16 | 19 | 19 | 22 | 26 | 29 | 34 | 38 | 10 | 9 | 11 | 12 | 16 | 18 | 18 | 21 | 20 | 2 | 1 | 4 |
| 500 | 500 | 14 | 16 | 18 | 19 | 21 | 27 | 29 | 33 | 36 | 11 | 10 | 13 | 16 | 15 | 15 | 17 | 19 | 19 | 2 | 2 | 4 |
| 600 | 600 | 22 | 25 | 29 | 30 | 34 | 35 | 39 | 41 | 44 | 14 | 15 | 11 | 19 | 24 | 26 | 20 | 25 | 26 | 3 | 3 | 3 |
| 800 | 800 | 37 | 41 | 46 | 48 | 52 | 55 | 57 | 57 | 60 | 22 | 26 | 27 | 29 | 34 | 37 | 39 | 44 | 45 | 5 | 4 | 6 |
| 950 | 950 | 42 | 42 | 46 | 47 | 58 | 60 | 66 | 68 | 68 | 28 | 29 | 28 | 31 | 33 | 39 | 42 | 46 | 49 | 4 | 4 | 4 |
| 1000 | 1000 | 42 | 43 | 47 | 50 | 51 | 59 | 61 | 65 | 69 | 34 | 33 | 35 | 30 | 35 | 39 | 49 | 52 | 55 | 5 | 6 | 3 |

*The number of detected but mismatched malware samples separately detected by both neural networks. These samples were output to a special dataset and verified by publicly available malware detection resources.

Table 4. Number of detected threats.

|  |  | The number of samples detected and classified as threats at different sizes ( $256,512,1024$ bytes) and three epochs (I, II, III) of training by a capsular neural network |  |  |  |  |  |  |  |  | The number of samples detected and classified as a threat at different sizes (20, 40, 128 bytes) and three epochs (I, II, III) of training by a convolutional neural network |  |  |  |  |  |  |  |  | Number of detected but mismatched malware samples * |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \mathrm{CTPI} \\ & \text { (by } \end{aligned}$ |  | 256 |  |  | 512 |  |  | 1024 |  |  | 256 |  |  | 512 |  |  | 1024 |  |  |  |  |  |
| $\begin{aligned} & \text { Trai } \\ & \text { ep } \end{aligned}$ |  | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III |
| 100 | 100 | 18 | 14 | 16 | 14 | 16 | 19 | 8 | 12 | 14 | 7 | 11 | 14 | 9 | 11 | 14 | 7 | 8 | 11 | - | 1 | 1 |
| 200 | 200 | 18 | 12 | 12 | 14 | 18 | 19 | 11 | 13 | 10 | 3 | 4 | 3 | 5 | 8 | 11 | 5 | 9 | 14 | 1 | 1 | 2 |
| 300 | 300 | 17 | 19 | 16 | 14 | 17 | 12 | 10 | 21 | 23 | 9 | 11 | 10 | 8 | 12 | 9 | 8 | 8 | 13 | - | 2 | 2 |
| 350 | 350 | 18 | 18 | 21 | 18 | 21 | 23 | 23 | 27 | 27 | 9 | 15 | 17 | 12 | 18 | 14 | 14 | 11 | 12 | 2 | 2 | 3 |
| 450 | 450 | 22 | 26 | 28 | 29 | 29 | 34 | 20 | 23 | 25 | 12 | 15 | 13 | 20 | 16 | 16 | 17 | 29 | 13 | 2 | 5 | 3 |
| 500 | 500 | 23 | 24 | 29 | 31 | 33 | 30 | 28 | 21 | 32 | 16 | 12 | 15 | 22 | 22 | 25 | 28 | 26 | 25 | 3 | 7 | 7 |
| 600 | 600 | 28 | 31 | 30 | 32 | 35 | 39 | 34 | 38 | 41 | 20 | 24 | 21 | 24 | 28 | 25 | 29 | 34 | 31 | 5 | 6 | 6 |
| 800 | 800 | 37 | 37 | 39 | 41 | 46 | 39 | 42 | 46 | 49 | 31 | 28 | 34 | 34 | 25 | 27 | 39 | 32 | 34 | 7 | 9 | 11 |
| 950 | 950 | 48 | 53 | 53 | 52 | 58 | 56 | 64 | 65 | 56 | 34 | 30 | 31 | 35 | 38 | 38 | 39 | 42 | 45 | 11 | 9 | 10 |
| 1000 | 1000 | 47 | 52 | 51 | 56 | 61 | 60 | 64 | 66 | 68 | 40 | 42 | 46 | 42 | 44 | 44 | 47 | 49 | 51 | 8 | 11 | 12 |

Fig. 6 shows a report from the virustotal service when examining one of the mimikatz malware samples detected by neural networks. In particular, the virustotal service did not detect either the file type or whether CTPH (based on ssdeep) belongs to a particular type of malware.


Fig. 6.Virustotal service report.

Tables 5 and 6 present the results of the studies of the operation of capsule and convolutional neural networks, based on data sets from the obfuscated compiled code of the mimikatz software.

Table 5. Number of detected threats.

|  | $\begin{aligned} & \text { Number of datasets } \\ & \text { (dataset 2) } \end{aligned}$ | The number of samples detected and classified as threats at different sizes (20, 40, 128 bytes) and three epochs (I, II, III) of training by a capsular neural network |  |  |  |  |  |  |  |  | The number of samples detected and classified as a threat at different sizes (20, 40, 128 bytes) and three epochs (I, II, III) of training by a convolutional neural network |  |  |  |  |  |  |  |  | Number of detected but mismatched malware samples * |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| CTPN size (byte) |  | 20 |  |  | 40 |  |  | 128 |  |  | 20 |  |  | 40 |  |  | 128 |  |  |  |  |  |
| Trai epo | $\begin{aligned} & \text { ing } \\ & \hline \end{aligned}$ | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III |
| 100 | 100 | 2 | 1 | 2 | 3 | 2 | 3 | 3 | 4 | 4 | 2 | 2 | 3 | 3 | 3 | 4 | 5 | 2 | 3 | - | - | - |
| 200 | 200 | 3 | 2 | 3 | 3 | 4 | 2 | 2 | 3 | 3 | 1 | 1 | 2 | 2 | 3 | 2 | 4 | 3 | 4 | - | - | - |
| 300 | 300 | 3 | 4 | 4 | 4 | 4 | 5 | 3 | 5 | 5 | 2 | 3 | 3 | 4 | 3 | 4 | 4 | 4 | 4 | - | - | 1 |
| 350 | 350 | 3 | 3 | 4 | 4 | 5 | 5 | 5 | 6 | 6 | 3 | 3 | 3 | 3 | 4 | 5 | 5 | 4 | 4 | - | 1 | 1 |
| 450 | 450 | 4 | 5 | 5 | 5 | 6 | 6 | 6 | 8 | 9 | 3 | 4 | 4 | 4 | 5 | 6 | 5 | 7 | 7 | - | 1 | - |
| 500 | 500 | 3 | 5 | 5 | 5 | 6 | 8 | 8 | 9 | 11 | 4 | 4 | 5 | 5 | 7 | 9 | 9 | 10 | 10 | - | 2 | 2 |
| 600 | 600 | 5 | 6 | 6 | 6 | 8 | 9 | 11 | 11 | 12 | 5 | 4 | 7 | 7 | 9 | 11 | 10 | 11 | 10 | 1 | 1 | 1 |
| 800 | 800 | 7 | 6 | 7 | 7 | 8 | 11 | 13 | 14 | 14 | 6 | 8 | 9 | 8 | 8 | 9 | 8 | 11 | 13 | 2 | 1 | 2 |
| 950 | 950 | 9 | 9 | 10 | 11 | 9 | 11 | 12 | 15 | 15 | 8 | 10 | 10 | 11 | 13 | 15 | 14 | 15 | 17 | 2 | 2 | 3 |
| 1000 | 1000 | 11 | 13 | 14 | 14 | 14 | 15 | 17 | 19 | 18 | 10 | 11 | 11 | 11 | 13 | 16 | 18 | 21 | 23 | 2 | 4 | 4 |

Table 6. Number of detected threats

|  |  | The number of samples detected and classified as threats at different sizes ( $256,512,1024$ bytes) and three epochs (I, II, III) of training by a capsular neural network |  |  |  |  |  |  |  |  | The number of samples detected and classified as a threat at different sizes ( $256,512,1024$ bytes) and three epochs (I, II, III) of training by a convolutional neural network |  |  |  |  |  |  |  |  | Number of detected but mismatched malware samples * |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| CTPN size (byte) |  | 256 |  |  | 512 |  |  | 1024 |  |  | 256 |  |  | 512 |  |  | 1024 |  |  |  |  |  |
| $\begin{array}{r} \text { Trair } \\ \text { epo } \\ \hline \end{array}$ |  | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III | I | II | III |
| 100 | 100 | 9 | 11 | 12 | 12 | 14 | 14 | 15 | 16 | 16 | 8 | 8 | 10 | 11 | 13 | 12 | 11 | 11 | 10 | - | - | 1 |
| 200 | 200 | 10 | 12 | 13 | 14 | 13 | 13 | 15 | 15 | 12 | 11 | 10 | 11 | 12 | 11 | 13 | 12 | 13 | 14 | - | 1 | 1 |
| 300 | 300 | 11 | 12 | 12 | 15 | 17 | 18 | 19 | 18 | 18 | 10 | 12 | 13 | 12 | 14 | 14 | 15 | 14 | 14 | - | - | - |
| 350 | 350 | 11 | 11 | 12 | 12 | 12 | 16 | 15 | 11 | 14 | 14 | 12 | 13 | 15 | 15 | 15 | 18 | 19 | 21 | - | 1 | 2 |
| 450 | 450 | 13 | 12 | 13 | 13 | 15 | 15 | 16 | 17 | 18 | 11 | 12 | 13 | 14 | 16 | 16 | 15 | 17 | 19 | 2 | 3 | 3 |
| 500 | 500 | 12 | 14 | 14 | 14 | 15 | 14 | 15 | 11 | 12 | 11 | 10 | 11 | 13 | 14 | 12 | 15 | 15 | 16 | - | 1 | 2 |
| 600 | 600 | 10 | 11 | 12 | 10 | 12 | 12 | 12 | 14 | 13 | 9 | 10 | 11 | 12 | 10 | 10 | 14 | 15 | 14 | 1 | 2 | 2 |
| 800 | 800 | 12 | 14 | 15 | 15 | 16 | 17 | 17 | 18 | 18 | 16 | 14 | 15 | 15 | 16 | 17 | 18 | 21 | 19 | 2 | 3 | 3 |
| 950 | 950 | 12 | 13 | 12 | 14 | 15 | 15 | 16 | 18 | 19 | 12 | 12 | 13 | 14 | 15 | 16 | 12 | 15 | 16 | 2 | 3 | 4 |
| 1000 | 1000 | 12 | 12 | 13 | 13 | 15 | 16 | 16 | 17 | 18 | 11 | 10 | 12 | 15 | 16 | 17 | 18 | 19 | 20 | 2 | 2 | 3 |

Given the malware source code (or fragment), the capsule neural network performs better than the convolutional neural network in detecting obfuscated malware. But when compiled, the detection performance of the capsular neural network decreases. Also, both neural networks separately detected a small set of data and software fragments classified as malware. Figures. [7]-[12] show a visualization of the output data of a capsule neural network with 3 training epochs and CTPN datasets, 20, 40, 80, 128, 256, 512 bytes.


Fig. 7. Visualization of malware detection results by capsule neural network.
(I training epoch, CTPH size 20 bytes)


Fig. 9. Visualization of malware detection results by capsule neural network. (II training epoch, CTPH size 80 bytes)


Fig. 11. Visualization of malware detection results by capsule neural network.
(III training epoch, CTPH size 256 bytes)


Fig. 8. Visualization of malware detection
by capsule neural network.
(I training epoch, CTPH size 40 bytes)


Fig. 10. Visualization of malware detection by capsule neural network.
(II training epoch, CTPH size 128 bytes)


Fig. 12. Visualization of malware detection results by capsule neural network. (III training epoch, CTPH size 512 bytes)

With an increase in the size of the CTPH files (interval 256, 512, 1024 bytes) for training the capsule network, the increase in the detection of the number of malware code fragments is insignificant ( $0.3-0.5 \%$, Fig. 7, Fig. 8, Table 6) in contrast to files $20,40,128$ bytes ( $12-14 \%$ increase). But increasing the size of the CTPH file allows increasing the editorial distance (Figure 9-12) to granularly group malware by type.

## 4. Conclusion

This paper proposes the use of transfer learning of a capsule neural network to detect obfuscated malware. Convolutional and capsule neural networks were trained on the same datasets. The source codes of mimikatz, athena, engrat, grum, surtr, dyre malware were used as datasets. When building an intrusion detection system using neural networks, their complex application is necessary. Annotated malware datasets are critical when training neural networks. The use of transfer learning of a capsule neural network to detect malware is justified if the source code of the malware or its fragments (preferably the first versions) is available. In this case, the neural network detects malware, even with its high degree of obfuscation. But in the absence of source code, the effectiveness drops, yielding to «standard» means of detecting malware. The use of the CTPH method for generating «weight» coefficients of a neural network is most effective with a small file size of CTPH.
Increasing the editorial distance increases the selectivity of detecting different types of malware.

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<br><br>e-mail: t.jamgharyan@yandex.ru

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# Исследование обфусцированного вредоносного программного обеспечения с помощью капсульной нейронной сети 

Тимур В. Джамгарян<br>Национальный политехнический университет Армении<br>e-mail: t.jamgharyan@yandex.ru


#### Abstract

Аннотация

Системы обнаружения и предотвращения вторжений являются неотьемлимым компонентом безопасности сетевой Инфраструктуры. Классические системы обнаружения и предотвращения вторжений не в состоянии обнаружить угрозу не описанную в наборе правил. Также нерешенной полностью задачей является: задача обнаружения вредоносного программного обеспечения подвергнутого обфускации. Исследователи в сфере безопасности программного обеспечения и сетевой Инфраструктуры пытаются решить данные задачи с помощью машинного обучения. В работе представлены результаты исследования использования трансферного обучения капсульной нейронной сети для обнаружения вредоносного программного обеспечения. Исследование проводилось на основе исходного кода вредоносного программного обеспечения с использованием метода контекстно-кусочного хеширования. Исходные коды вредоносного программного обеспечения были получены из общедоступных источников программного обеспечения. Проверка результатов обучения капсульной нейронной сети проводилась с использованием обученной сверточной нейронной сети и общедоступных источников тестирования вредоносного программного обеспечения. Исходные коды разработанного программного обеспечения, часть наборов данных для обучения нейросети, результаты исследования не внесенные в статью представлены по адресу https://github.com/T-JN

Ключевые слова: капсульная нейронная сеть, нечеткое хэширование, система обнаружения вторжений, редакционное расстояние, трансферное обучение.


# Data Processing and Persistence in Virtual Reality Systems 

Arman A. Hovhannisyan<br>National Polytechnic University of Armenia<br>e-mail: aahovhannisyan1@gmail.com


#### Abstract

Data processing and persistence are key aspects of developing a Virtual Reality system. In this paper, an improvement is offered to the distance calculation algorithm of the Unity Engine. Additionally, data persistence mechanisms provided by the Unity Engine are reviewed, and File System is selected as an appropriate option. Storage of object coordinates to the File System is implemented. The results provide a baseline for developing a system for creating virtual stands for professional research.


Keywords: Virtual reality, Data management, File System, Serialization.
Article info: Received 29 March 2022; received in revised form 9 October 2022; accepted 17 November 2022.

## 1. Introduction

In virtual reality, data is represented both in primitive types (int, float, string) and complex types provided by the engine. Object positions in space are determined in the Cartesian coordinate system [1] (see Fig. 1).

A common task is to compare the distance of 2 points from a given point $A\left(x_{1}, y_{1}, z_{1}\right)$. The Unity Engine Scripting API [2] provides a complex data type called Vector3 to store object coordinates, along with its Vector3.Distance() method to calculate distance between 2 points. Given the points $\left(x_{2}, y_{2}, z_{2}\right), C\left(x_{3}, y_{3}, z_{3}\right)$, this method may be used to accomplish the task, comparing the following values: Vector3.Distance(B, A), Vector3.Distance(C, A). A more efficient solution may be applied using the formula of the distance between 2 points [1]:

$$
\begin{equation*}
d_{A B}=\sqrt{\left(x_{2}-x_{1}\right)^{2}+\left(y_{2}-y_{1}\right)^{2}+\left(z_{2}-z_{1}\right)^{2}}, \tag{1}
\end{equation*}
$$

$$
\begin{equation*}
d_{A C}=\sqrt{\left(x_{3}-x_{1}\right)^{2}+\left(y_{3}-y_{1)}^{2}+\left(z_{3}-z_{1}\right)^{2}\right.} \tag{2}
\end{equation*}
$$

Instead of comparing values for $d_{A B}$ and $d_{A C}$, the radicands may be compared, saving CPU time on unnecessary calculations.


Fig. 1. Object positions in space.
To have persistent data between sessions, the user progress has to be stored on the disk. There are several methods of managing data storage, including SQL database, PlayerPrefs and OS File System. On specific events during the runtime, which are to be defined, data containing all the current values have to be stored. These events may include user interaction, object state mutation, or events may be set to trigger on specific timestamps, e.g., every 10 seconds. Then, on the next program run, these stored values have to be fetched and transmitted to the engine to render the objects in the same state and position, as they were when the last event was triggered.

## 2. Persistent Data

To have persistent data between sessions, the user progress has to be stored on the disk. Below are listed several methods of managing data storage.

## 1. SQL Database

SQL is useful when there is relational data. It supports queries to fetch related data sets. In our case, we have just objects that need to be memorized and then retrieved on the next run. Such simple operations are easier to implement and faster in work on File System. SQL is a dedicated software and isn't an integrated part of Operating Systems, as File System is. Also, a connection to SQL service should be kept active during the runtime.

## 2. PlayerPrefs

PlayerPrefs is a class provided by Unity Engine that stores Player preferences between game sessions. It stores values in the OS registry. Though it is possible to store data using this
method, it is not recommended to do so. This method should be used for data, that can be afforded to lose, such as user settings and preferences. Sensitive and relatively big data should not be kept in registries.

## 3. File System

To store data in files, it needs to be formatted in some way. It may be serialized [3] to binary format and written to a file. That data will then be successfully deserialized and used in the application. But since binary is not human-readable, it makes this format insufficient. Moreover, it is not possible to edit the saved data manually. Using JSON data type allows bypassing these problems.

Taking into account the points mentioned above, it was decided to handle data storage using File system and Serialization, so every time data needs to be stored, it is serialized to JSON format and written to a file (see Fig. 2). Then, to restore the state in the application, the file is read and data is deserialized to object (see Fig. 3).


Fig. 2. Storing Data.


Fig. 3. Using Stored Data.

## 3. Saving Object Position

A specific and common example is persisting the object position. In this example, we have a cube placed on a table (see Fig. 4). The Origin ( $0,0,0$ ) can be located on the ground.


Fig. 4. Cube.

To save the cube position after it is replaced, a class called SaveManager is created, which contains 2 methods: save and load. These methods use a file called "position.dat" to write/read data.
SaveManager.cs
public class SaveManager
\{
public static void save(Vector3 pos)
\{
string path = Path.Combine(Application.persistentDataPath, "position.dat"); File.WriteAllText(path, JsonUtility.ToJson(pos));
\}
public static Vector3 load()
\{
string path = Path.Combine(Application.persistentDataPath, "position.dat");
string result = File.ReadAllText(path);
Vector3 pos = JsonUtility.FromJson<Vector3>(result);
return pos;
\}
\}
The save and load methods would then be invoked from a script, which is bound to the object. The save method would be bound to the XR Grab Interactable component [4] "Select Exited" event to save data every time the object is released. The load method would be invoked from the Start method to set object positions from the saved data on a fresh program run.
CubeScript.cs
public class CubeScript : MonoBehaviour
\{
// Start is called before the first frame update
void Start()
\{
Vector3 position = SaveManager.load();
transform.position = position;
\}
public void Save()
\{
SaveManager.save(transform.position);
\}
\}


Fig. 5. Cube position changed via left controller.
The saved file position.dat:
\{"x":-0.0030583017505705358,"y":0.838373601436615,"z":-2.0934112071990969\}
After restarting the program, we still have the cube in its new place (see Fig. 5).
Now we can modify this file content, and set the coordinates to ( $0,0,0$ ).
\{"x":0,"y":0,"z":0\}
After modifying and saving the file, and running the program again, we can see that the cube appears on the Origin as expected (see Fig. 6).


Fig. 6. Cube position manually set to Origin.

## 4. Conclusion

In this article, an improvement to the Unity Engine distance calculation algorithm was suggested. Additionally, data types provided by the Unity Engine were reviewed. Data storage options were compared and decided to use the OS File System and data serialization. As an example, a cube position storage and loading were implemented. This method will be used also for custom complex data types to store, marking the class representing the data type as Serializable.

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Upưuí U. Zņhuikihujuí<br><br>e-mail: aahovhannisyan1@gmail.com

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# Обработка и сохранение данных в системах виртуальной реальности 

Арман А. Оганесян<br>Национальный политехнический университет Армении e-mail: aahovhannisyan1@gmail.com


#### Abstract

Аннотация

Обработка и сохранение данных являются ключевыми аспектами разработки системы виртуальной реальности. В данной статье предлагается улучшение алгоритма расчета расстояний Unity Engine. Кроме того, рассматриваются механизмы сохранения данных, предоставляемые Unity Engine, и в качестве подходящего варианта выбирается файловая система. Реализуется хранение координат объекта в файловой системе. Результаты обеспечивают основу для разработки системы создания виртуальных стендов для профессиональных исследований.

Ключевые слова: Виртуальная реальность, управление данными, файловая система, сериализация


# Network Management Automation Through Virtualization 

Arusyak D. Manasyan<br>Institute for Informatics and Automation Problems of NAS RA<br>e-mail:armanasyan@iiap.sci.am


#### Abstract

The study aims to develop methods for automating network management by analyzing its virtual counterpart. The paper substantiates the relevance of this approach, identifies the advantages and disadvantages, highlights the existing problems, and suggests ways to solve them. As a result, the effectiveness of network virtualization was shown by the example of an experimental network.


Keywords: network, automation, virtualization, SDN (Software-Defined Network), OpenDaylight (Software), OpenFlow (Protocol).
Article info: Received 10 December 2021; received in revised form 8 July 2022; accepted 23 August 2022.

## 1. Introduction

The more devices are connected to the network, the more inconvenience there will be with the expenses of their utilization. And until the network system is automated, this problem will be constant. Organizations will spend a lot of money to buy powerful network devices, but network management will not become easier. That is why a study of network automation and virtualization was carried out, their current applications were discussed and solutions to existing problems were proposed.

As network traffic continues to grow, companies increasingly require large-scale network configurations. The move to cloud computing continues as enterprise customers and their applications rely more and more on network efficiency, so networks are expected to be highly reliable with minimal downtime. As the number of devices on the network increases, so does the need for uninterrupted, flexible, fast, and efficient communication between them. To do this, it is necessary to obtain a large number of network devices that will be of a high quality, and have great features, such as a large amount of memory, many interfaces, and powerful processors, and all this is associated with high costs, which is one of the main prerequisites for the emergence automation and virtualization concepts.

For service providers, automation is a key strategy to improve network agility and reliability while controlling operating and capital costs. Therefore, it is necessary to automate the work
with network equipment. Automation of daily network tasks and functions, as well as automated monitoring of iterative processes, increases the availability of network services.

We can describe the current state of the networking industry as "critical". The marketdominant closed (proprietary) solutions are "boxes" for applications, and the interoperability of solutions from different vendors is best provided at the interface level. Networks are extremely complex, making them difficult to scale, manage, and trust. This slows down the further development of networks and programs running in them. Therefore, several solutions for network automation have been developed, and we talked about SDN in our research work. Software Defined Networking (SDN) introduces network virtualization capabilities, which makes it easier to build and manage network automation tasks. Using SDN, networks can be provisioned at the software layer, abstracting the underlying physical hardware. This takes automation to the next level and significantly accelerates network provisioning and configuration management. It also enables IT to attach network and security services to workloads using a policy-driven approach(see [1]). Today, network automation solutions allow us to perform a wide range of tasks, including network planning - design, including scenario planning - backup management, device testing - configuration testing, deployment of deployed physical devices services, as well as virtual device deployment - provisioning devices, real-time network data collection systems related to applications, network topology, traffic, services, data analysis, including active artificial intelligence, machine learning analysis, to get an idea of the present and future, network behavior, check configuration compliance, to ensure all network devices and service requirements, software updates, including backing up software if necessary, fixing closed network issues, including troubleshooting, and complex, difficult-to-detect Troubleshooting activities, detailed analysis of reports, panels, alarms, warnings, compliance with security requirements, monitoring of the network and its services, service level to maintain customer satisfaction.

The purpose of this article is to show the benefits of network virtualization, present the tools necessary for this, and show its effectiveness as a result of the experimental application.

## 2. Analyses and Discussion

Network automation through SDN (see [2]) adds a number of capabilities to conventional automation paradigms, which optimize IT resources and require SDN as a networking architecture approach. It enables the control and management of networks using software applications. Through SDN networking, the behavior of the entire network and its devices is programmed in a centrally controlled manner through software applications using open APIs. SDN improves performance through network virtualization. In SDN ${ }^{[2]}$ software-controlled applications or APIs work as a basis of complete network management that may be directing traffic on a network or communicating with underlying hardware infrastructure. So to put it simply, we can say that SDN can create virtual networks or control traditional networks with the help of software to improve security and reduce cost.

Traditional network refers to the old conventional way of networking, which uses fixed and dedicated hardware devices such as routers and switches to control network traffic. Inability to scale, as well as network security and performance are major concerns nowadays in the current growing business situation so SDN is taking control of traditional networks. The traditional network is static and based on hardware network appliances. Traditional network architecture was used by many companies until recent years but nowadays due to its drawbacks SDN has been developed and will be used more widely in the coming years(see [3]).

Table 1. Comparison of SDN to Traditional Network(see [3]).

| No | SDN | Traditional Network |
| :---: | :---: | :---: |
| 1 | Virtual networking approach. | Old conventional networking approach. |
| 2 | Centralized control. | Distributed control. |
| 3 | Programmable network. | This network is nonprogrammable. |
| 4 | Open interface. | Closed interface. |
| 5 | Data plane and control plane are <br> decoupled by software. | Data plane and control plane are mounted on <br> the same plane. |
| 6 | It supports automatic configuration <br> so it takes less time. | It supports static/manual configuration so it <br> takes more time. |
| 7 | It can prioritize and block specific <br> network packets. | It leads all packets in the same way with no <br> prioritization support. |
| 8 | It is easy to program as per need. | It is difficult to program again and replace the <br> existing program as peruse. |
| 9 | The cost is low. | The cost is high. |
| 10 | Structural complexity is low. | Structural complexity is high. |
| 11 | Extensibility is high. | Extensibility is low. |
| 12 | It is easy to troubleshoot and report <br> as it is centralized and controlled. | It is difficult to troubleshoot and report as it is <br> distributed and controlled. |
| 13 | Its maintenance cost is lower than <br> the traditional network. | Cost is higher than SDN. |

As the SDN technology (see [4]) is based on an intelligent controller, it allows you to automatically redistribute traffic. It turned out that the device allows you to centrally change the settings of network equipment in branches, monitor the network status, load and quality of channels online, and solve problems. This ensures the transparency of data transmission networks and reduces the burden on IT professionals serving the network.

The study also showed that the SDN solution involves the automatic networking of private networks and the transmission of information through all available channels without losing the speed and quality of applications. For example, in the past, only expensive VPN channels were used to transmit audio or video without distortion. Now, thanks to SDN, we can only use the Internet and LTE as a backup(see [5]). In this way, customers can save on telecommunication bill payments and solve VPN reservation issues simply and cheaply. Unlike other virtualization technologies, the open-source SDN solution is more promising. $\mathrm{SDN}^{[2]}$ already provides companies with many options to choose from OpenFlow, NETCONF, OVSDB, switches that support the API library, as well as enterprise software that utilizes these protocols. Like any other infrastructure, the SDN infrastructure is built on open standards. This open ecosystem accelerates network innovation. Although the traditional approach to building a network infrastructure still prevails due to the negative impact of mental inertia and crisis events, SDN already allows you to effectively solve problems in a virtual physical environment.

By automating the network, we get the following benefits and services: reduced problems, reduced costs, increased network flexibility, reduced network outages, increased number of strategic employees, advanced analysis, and network management capabilities.

## 3. Methods and Applications

The article methodology includes the study of epistemological issues, programs (OpenDaylight), protocols (OpenFlow) in the field of networks, using scientific literature, and research articles.

The research aim is to present an example of an automated network as a result of the analysis based on the studied materials. Below is the physical experimental network represented by the GNS3 simulator, which is fully operational, we will get the virtualized version of the following network, but the initial settings must be done one way or another.

This article provides a brief overview of virtual networks and network performance evidence. The physical network shown below is represented by a fully running GNS3 simulator. It contains hosts, routers (Mikrotik), and a virtual switch - OpenvSwitch.


Fig . 1. Network presented with GNS3 simulator.

Here are the settings of one of the devices, almost the same as the rest:
/routing OSPF instance
set [ find default=yes ] router-id=10.255.255.1
/IP address
add address=10.0.4.1/24 interface=ether 4 network=10.0.4.0
add address $=192.168 .10 .1 / 24$ interface=ether3 network=192.168.10.0
/routing OSPF network
add area=backbone network=10.0.4.0/24
add area=backbone network=192.168.10.0/24
Here are the minimum settings that make the network complete.
For network virtualization, as mentioned at the beginning, we implemented an SDN solution. We have demonstrated the use of SDN with the OpenDaylight software, which is a software platform for SDN.

To work with our controller, to connect it to our physical network, we downloaded and activated the following components:
opendaylight-user@root>feature:install odl-restconf odl-l2switch-all odl-mdsal-apidocs odl-dlux-all odl-openflowplugin-all

They provide a graphical user interface of OpenDaylight software, as well as the necessary tools and devices. After activating them, immediately after setting the appropriate settings in our physical OpenvSwitch network, we see a virtualized version of our network.
To establish a "controller" connection in our physical network, we have previously configured the OpenvSwitch OpenFlow device by giving it the IP address of the controller by typing the following command: ovs-vsctl set-controller br0 tcp: 192.168.18.129:6633, where 192.168.18.129 is the IP address of the controller and it can be different for different devices, 6633 is the connection port and the protocol that controls data transfer over TCP. Thanks to this, it was able to communicate with other devices.


Fig. 2 . Example of a virtual network in OpenDaylight.
Fig. 2 shows a virtualized version of the physical network in OpenDaylight. The picture clearly shows all the devices in our network that are connected to the OpenFlow protocol support device, OpenvSwitch. It is thanks to the OpenFlow protocol that our SDN controller sees our entire physical network.

OpenFlow is a protocol for managing data processing, which is transmitted over the network through routers and switches using SDN technology. Fast packet forwarding (data forwarding) on a classic router or switch and high-level routing decisions (control operations) are made on the same device. The OpenFlow switch separates these two functions. Data redirection is performed by the switch itself, while routing decisions are entrusted to a separate controller, usually a standard server.
After clicking on the network topology, Yang automatically shows us the CONFREST API URL it uses to get this information:


Fig. 3. CONFREST API URL

By clicking the send button(Fig.3), we can see the topology of our operational network.


Fig. 4. Operating network topology.
In Fig. 4, we can see information about our current topology, including the MAC (Media Access Control) and IP addresses of our hosts. So, you do not need to enter the device to see them every time, but you can see them from one control panel of SDN.
When we send network traffic, all the information about it is mentioned in the flow tables of the SDN: how many packages were sent to us, how many arrived, how many dropped on the way, and what errors we encountered. And all that information we can see in the nodes of Fig.5.


Fig.5. Node connector statistics.

## 5. Conclusion

This paper proposes a solution for network optimization. As a result of the research, we concluded that automation improves the speed of IT operations in response to analytical change. The ability to monitor operations, just as needed, provides greater visual control of the network, and transparency of processes within it. Network automation improves work efficiency, reduces human error, increases access to network services, and provides better customer service. Research has shown that the SDN solution includes the automatic integration of private networks, and the transmission of information over all available channels, without loss of application speed and quality. As a result of the study, it became clear that network automation can be implemented regardless of its type, which facilitates its transition. Network virtualization is a more all-encompassing version of virtualization that makes it possible to convert physical network hardware into software that can easily be transitioned to different domains as needed, increasing flexibility and scalability for the network. I came to the conclusion that its use on the network will be of great benefit to network administrators.

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Upnıujulq ᄀ. Uuiduaujuis<br><br>e-mail:armanasyan@iiap.sci.am

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## Автоматизация управления сетью за счет виртуализации

Арусяк Д. Манасян<br>Институт проблем информатики и автоматизации НАН РА<br>e-mail:armanasyan@iiap.sci.am


#### Abstract

Аннотация

Цель исследования заключалась в разработке методов автоматизации управления сетью путем анализа ее виртуального аналога. В работе обосновывается актуальность такого подхода, выявляются преимущества и недостатки, подчеркиваются существующие проблемы и предлагаются пути их решения. В результате была показана эффективность виртуализации сети на примере пилотной сети.

Ключевые слова: сеть, автоматизация, виртуализация, SDN (Программноопределяемая сеть), OpenDaylight (Программное обеспечение), OpenFlow (Протокол).


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Unnpuqnıư $\hbar$ unuwqnnıpjuí 25.11.2022 Onıŋрฉ oqutip:<br> <br><br> Epluwa, T. Uluwlh 1 Zhn. +(374 60) 623553<br>qhin` wiul Kun

Подписано в печать 25.11.2022
Офсетная бумага.
Опубликовано Институтом проблем информатики и автоматизации НАН РА

Объём: 100 страниц. Тираж: 100
Лаборатория компьютерной
полиграфии ИПИА НАН РА.
Ереван, П. Севака 1
Тел.: +(374 60) 623553
Цена: бесплатно

Signed in print 25.11.2022
Offset paper
Published by Institute for Informatics and Automation Problems of NAS RA

Volume: 100 pages
Circulation: 100
Computer Printing Lab of IIAP NAS RA
Yerevan, 1, P. Sevak str.
Phone: +(374 60) 623553
Free of charge

