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Original scientific paper

#### ALTITUDE AND VEGETATION EFFECTS ON EPIGAEIC ARTHROPOD FAUNA FROM BELASICA MT. (SOUTH-EAST MACEDONIA) RUNNING TITLE: COMMUNITY STRUCTURE OF EPIGEIC MACROFAUNA ON BELASICA MT.

#### Aleksandra Cvetkovska-Gjorgjievska<sup>\*</sup>, Dana Prelić, Slavčo Hristovski, Valentina Slavevska-Stamenković, Milica Ristovska

Institute of Biology, Faculty of Natural Science and Mathematics, Ss. Cyril and Methodius University, Skopje, Republic of N. Macedonia

\*e-mail: <u>acgorgievska@yahoo.com</u>

Community structure of epigaeic arthropods along altitudinal gradient on Belasica Mountain was analysed. 140 pitfall traps were placed along a transect line at 14 sampling sites in the period April-November 2010. Altogether 6189 specimens were captured, belonging to 122 taxa (99 species and 23 morphospecies), 62 families, 14 orders and 5 classes. The largest contribution within fauna had beetle community (Coleoptera - 110 speices). Most numerous as expected were Coleoptera (44.76 %) and Araneae (32.47 %), followed by Diplopoda (7.86 %), Opiliones (5.97 %) and Isopoda (3.57 %).

The increasing altitude and differences of vegetation type (oak to beech forests) along the gradient influenced community structure with significant increase of the overall arthropod relative abundance. The highest relative abundance was registered in a submontane beech forest (1100 m a.s.l), while the lowest value was obtained in the locality dominated by the sessile oak forest (587 m a.s.l). The relative abundance of Aranea, Coleoptera, Diplopoda, Chilopoda, Microcoryphia and Blattodea increased with the elevation and significantly differed between localities and vegetation types, as well. Unlike them, the relative abundance of Scorpiones, Opiliones and Isopoda, significantly decreased along the gradient and consequently with differences of vegetation type. In contrast to the relative abundance, the overall species richness was influenced only by the increasing altitude.

Key words: epigaeic arthropods; elevation effects; Belasica Mt.; vegetation types

#### INTRODUCTION

Knowledge about ecosystem functioning and arthropod reactions to environmental changes is of conservation importance, especially in high mountain areas [10] and among other reasons especially because of the climate changes. According to [15] the studies documenting the present day altitudinal distribution of plants and animals will be an irreplaceable source for the estimation of ecological global warming effects. Additionally, to better understand biodiversity changes in mountainous ecosystems it is important to study how organisms are influenced by elevation and how they response to those changes.

Arthropods comprise many different functional guilds and are sensitive indicators of changes in environmental conditions [13]. Hence the aim of this study was to obtain basic knowledge of arthropod fauna, emphasizing their species richness, abundance and distribution range along altitudinal gradient at the northern part of Belasica Mt The boundary position of the mountain, the autochthonic plant communities and the influence of Mediterranean climate contributes to forming the complexes of many faunal, biogeographical and ecological elements of arthropod fauna.

The long term studies will improve the existing knowledge of epigaeic macrofauna on Belasica Mountain and further on other mountainous ecosystems in Republic of Macedonia.

#### MATERIAL AND METHODS

#### Area of research

Belasica Mountain is situated at the south-east part of Macedonia, bounded between Bulgaria and Greece (Figure 1). It belongs to the group of high mountains (over 2000 m) [6] and is among the smallest by area mountains in Macedonia. Belasica was formed as a mountain block during the Pliocene between two parallel seedlings bounded from north and south, rising as a horst between two sinking anticlinoria.

The mountain is build up mainly of metamorphic rocks–amphibolites, different types of minerals, granite, gneiss etc. Low parts of the mountain are characterized with cinnamon-forest soils, and at the higher parts most common are brown-forest and mountain-meadow soils. Climate in the lowmountain belt (300–1000 m) is mountain continental with Mediterranean influence, while the mountain belt over 1000 m alt. is influenced by the cold continental climate [7].



Figure 1. Topographic map of the investigated area and localities on Belasica Mountain

#### Sampling design

Fourteen localities (L1–L14) at different altitudes (240–1450 m a.s.l.) along an altitudinal gradient were selected at the north part of Belasica Mountain.

The vegetation cover is represented by several climazonal forests: first five localities (L1–L5) are covered by the association *Querco-Carpinetum orientalis macedonicum* Rudski apud Ht – Qqo (White oak and Oriental hornbeam); L6–L9 are dominated by the association *Orno-Quercetum petraeae* Em - Oqp (Sessile oak); L10 is disposed within the association *Festuco heterophyllae-Fagetum* - Fhf (Submontane beech forest); L10–L13 are allocated within the association *Calamintho grandiflorae-Fagetum* - Cgf (Montane beech forest), and L14 representing clear-cut area in a mountain beech forest.

The material was collected with pitfall traps placed along a 100 m long transect line. In each locality, one set contained of 10 pitfall traps was placed and traps were spaced 10 m apart from each other. In total 140 traps were placed in 14 different localities (L1–L14) referring to different altitudes on Belasica Mountain. Plastic cups were used as pitfall traps (volume of 0.5 L, diameter of 8.5 cm and height of 11.5 cm) and covered with metal raincover. Formaldehyde-vinegar solution (1:7; 200 ml) was used as a preservative. As pitfall-trapping is most appropriate method for collections of grounddwelling fauna [17, 18], most of the samples were active dwellers on the soil surface and only those representatives were considered in the analysis.

The material was collected monthly, at the end of the month in the period April-November 2010. Data about the localities are presented in Table 1.

Code	Altitude (m)	Locality	GPS coordinates	Slope (%)	Vege- tation cover (%)
L1	250 a.s.l.	near the locality of Markova Skala; ass. <i>Querco-Carpinetum</i> orientalis macedonicum Rud. 1939 ap. Ht. 1946	41°22'6.34"N 22°48'4.54"E	70	80
L2	327 a.s.l.	under the viewing point near the Koleshino Waterfall; ass. <i>Querco-Carpinetum orientalis macedonicum</i> Rud. 1939 ap. Ht. 1946	41°22'37.62"N 22°48'46.14"E	70	85
L3	415 a.s.l.	near the Koleshino Waterfall; ass. <i>Querco-Carpinetum</i> orientalis macedonicum Rud. 1939 ap. Ht. 1946	41°22'17.82"N 22°48'25.38"E	15	90
L4	500 a.s.l.	near the locality of Pod; ass. <i>Querco-Carpinetum orientalis</i> macedonicum Rud. 1939 ap. Ht. 1946	41°22'12.90"N 22°48'25.38"E	70	50
L5	587 a.s.l.	between the localities of Pod and Suva Cheshma ass. <i>Querco-Carpinetum orientalis macedonicum</i> Rud. 1939 ap. Ht. 1946	41°22'6.34"N 22°48'4.54"E	10	60
L6	693 a.s.l.	near the locality of Suva Cheshma; ass. Orno-Quercetum petraeae Em 1968 (Fraxino orni-Quercetum petraeae Em 1968)	41°22'3.87"N 22°48'13.20"E	40	90
L7	767 a.s.l.	near the locality of Popadija; ass. Orno-Quercetum petraeae Em 1968 (Fraxino orni-Quercetum petraeae Em 1968)	41°22'0.88"N 22°48'8.80"E	25	70
L8	847 a.s.l.	near the locality of Popadija; ass. Orno-Quercetum petraeae Em 1968 (Fraxino orni-Quercetum petraeae Em 1968)	41°22'0.88"N 22°48'8.80"E	15	90
L9	1038 a.s.l.	near the locality of Popadija; ass. Orno-Quercetum petraeae Em 1968 (Fraxino orni-Quercetum petraeae Em 1968)	41°22'0.88"N 22°48'8.80"E	20	95
L10	1100 a.s.l.	near the locality of Popadija; ass. <i>Festuco heterophyllae-Fagetum</i> (Em 1965) Rizovski & Džekov ex Matevski et al. 2011	41°22'0.88"N 22°48'8.80"E	25	85
L11	1200 a.s.l.	near the locality of Popadija; ass. <i>Calamintho grandiflorae-Fagetum</i> (Em 1965) Rizovski & Džekov ex Matevski et al. 2011	41°22'0.88"N 22°48'8.80"E	60	90
L12	1300 a.s.l.	near the locality of Groba; ass. <i>Calamintho grandiflorae-</i> <i>Fagetum</i> (Em 1965) Rizovski & Džekov ex Matevski et al. 2011	41°22'0.88"N 22°48'8.80"E	60	90
L13	1385 a.s.l.	near the locality of Pisana Skala; ass. <i>Calamintho grandiflo- rae-Fagetum</i> (Em 1965) Rizovski & Džekov ex Matevski et al. 2011	41°22'16.55"N 22°48'13.88"E	45	60
L14	1442 a.s.l.	near the locality of Pisana Skala; clear-cut area	41°22'0.88"N 22°48'8.80"E	25	60

**Table 1.** List of the investigated localities with the data about the altitudes,

 GPS coordinates slope and dominant vegetation type

#### Data analyses

Most of the arthropod specimens were identified to a morphospecies level. The specimens of orders Araneae, Chilopoda and Diplopoda were identified only to a family level. The exceptions are major part of order Coleoptera representatives identified to a species level, and only those specimens identified to a species and morphospecies level were included in the species richness analysis, while quantitative analyses were applied to all registered groups, including those identified to a family level.

Species richness and relative abundance were analyzed for each altitude and vegetation type along the gradient, and adult as well as larval stages were considered.

The relative abundance was represented as number of individuals per trap (ind.trap<sup>-1</sup>). Dominance of species was calculated as a percentage of the number of individuals of a species in a total

number of individuals of all species. Regarding their dominance species were classified in four groups: dominant species (D) over 10 %, subdominant species (SD) -5-10 %, recedent species (R) -1-5 % and subrecedent species (SR) - with the occurrence less than 1 % (Balogh 1958).

Shapiro-Wilks and Levene's tests were used to analyze the normality of distributions and homogeneity of variance, respectively. For normal distribution, data were log(x+1) transformed. But, because neither normal distribution nor homogeneity of the variance were recorded after the normality test was applied, non-parametric tests were applied: the nonparametric test Kruskal Wallis ANOVA as an analogue test of ANOVA and the post-hoc test Mann-Whithey U (which follows in cases where significant differences are recorded with the Kruskal Wallis ANOVA test). These tests were applied to check for the differences in average species richness and abundance within and between localities and vegetation types. These results are presented with box plots.

Spearman rank correlation (r) test was used to analyze the relationship between the altitude and species richness as well as average abundance of captured specimens.

All statistical data analyses were done with statistical program STATISTICA 6 for Windows. Significant values were those with p<0.05.

#### **RESULTS AND DISCUSSION**

The epigaeic arthropod fauna along the altitudinal gradient on northern slopes of Belasica Mountain was represented by 6189 individuals of 99 species and 23 morphospecies, belonging to 5 classes, 14 orders and 62 families. Among them, Insecta was represented with four orders (Coleoptera, Dermaptera, Blattodea, Microcoryphia), the class Arachnida with three (Opiliones, Scorpions and Araneae), two classes of Myriapoda (Chilopoda and Diplopoda) were present with six orders and the class Malacostraca was presented with one order only (Isopoda). The largest contribution had beetle community (Coleoptera - 110 species).

Considering the fact that the pitfall trapping method is associated with the underestimation of the abundance of flying (Diptera – 8.86 %, Hymenoptera – 3.64 %, Homoptera – 1.16 %, Lepidopera – 0.76 %, Orthoptera – 0.31 %, Hemiptera – 0.21 %, Neuroptera – 0.0033 %, Mantodea – 0.0016 %, Mecoptera – 0.0016 %), small sized (Collembola – 33.62 %, Acarina – 3.61%, Pseudoscorpiones – 0.33 %), larval stages (larvae of Lepidoptera – 1.85 %, Diptera – 0.62 %, Hymenoptera – 0.11 %, Neuroptera – 0.01 %) and slowly moving epigaeic representatives (Oli-

gochaeta – 0.26 %, Gastropoda – 0.03 %), the same were excluded from the comparative analyses.

Although considerable differences of overall arthropod **species richness** between different forest types were not registered, the increasing altitude influenced community structure with decrease of species richness (r = -0.190, p < 0.05) throughout the gradient. Highest species richness (79) was registered in L6 (693 m a.s.l.), and the lowest (27) in L9 (1030 m a.s.l.), both localities dominated by sessile oak forest (Figure 2, A, B).

Low species richness in L9 was probably due to the lowest number of coleopteran species, while in general higher species richness in oak forests at lower altitudes is expected due to the favorable environmental conditions [1,3,4], often associated with higher temperature, as well as because of the greater habitat heterogeneity. According to [8], litter volume also, provides specific environmental conditions for epigaeic arthropods.



Figure 2. Average species richness of arthropod fauna a long altitudinal gradient A. and between different vegetation types B. on Belasica Mt.

Similar results were obtained by [16] in the research of diversity and abundance of soil invertebrates along an altitudinal gradient in the Silesian Beskid Mts (Western Carpathians), where diversity tended to decrease with altitude, and sites at higher elevations were poorer in invertebrate taxa.

The species richness of different arthropod groups did not change significantly along the gradient, neither with differences of vegetation structure along the same gradient. According to [21], changes of the species richness along the gradients vary depending on the taxonomic group that is studied.

The **relative participation** (%) of the specimens belonging to different arthropod groups is given on Figure 4. Most numerous as expected were Coleoptera (44.76 %) and Araneae (32.47 %), followed by Diplopoda (7.86 %) and Opiliones (5.97 %). Other representatives: Isopoda (3.57 %), Scorpiones (1.82 %) and Chilopoda (1.55 %) had recedent participation within the total arthropod fauna,

and the remaining groups appear subrecendent with participation less than 1 % (0.99 % -0.01 %).

The research of arthropod fauna showed significant differences of overall relative abundance between different forest types (r = 0.300, p < 0.05) and along the gradient (r = 0.298, p < 0.05), with significant increase throughout the same. Total arthropod abundance was higher in the localities from the upper altitudinal belt (L7–L14) especially in L9 (1038 m a.s.l.) and L14 due to the high relative abundance of spiders and L10 (1100 m a.s.l.) and L11 (1200 m a.s.l.) as a result of a high number of coleopterans. The highest relative abundance was registered in a submontane beech forest (Fhf) - L10 (1100 m a.s.l), while the lowest value was obtained in L5 (587 m a.s.l) dominated by sessile oak forest (Qgo) (Figure 3.A, B). In addition, [12], found that arthropod species richness and number of specimens in oak forests from northern Trace (Turkey) increased with elevation, also.



Figure 4. Relative participation (%) of different arthropod groups on Belasica Mt.

The relative abundance of Aranea (r = 0.435, p < 0.05), Chilopoda (r = 0.202, p < 0.05), Diplopoda (r = 0.473, p < 0.05), Microcoryphia (r = 0.243, p < 0.05), Coleoptera (r = 0.200, p < 0.05) and Blattodea (r = 0.335, p < 0.05) increased with the elevation and significantly differed between localities (Tab. 2) and vegetation types (Tab. 3). Coleoptera larvae also dominated at higher altitudes. The increased abundance of arthropods along the gradient was probably due to the low competition rate at higher altitudes. The abundance of spiders depends of the prey availability [14] which was probably more available at higher altitudes. With the exception of few localities dominated by the oak forests where their presence is recorded, microcoryphians occurred in higher abundance in the localities of the upper altitudinal belt. The same applies to Blattodea and to a certain level for centipedes whose abundance was higher in the upper part of the gradient. Millipedes preferred sub-mountain and mountain beech forests, but reached their highest values in the clear-cut area. Probably the milliped fauna from the clear-cut area is distinguished with different species composition from the previous, with domination of species which prefer more insolate and xeric condition. Identification on a species level is necessary in order to see which species determine the dynamics of the whole myriapod community.

The abundance of Scorpiones (r = -0.693, p < 0.05) Opiliones (r = -0.208, p < 0.05) and Isopoda (r = -0.241, p < 0.05), significantly decreased along the gradient (Tab. 2) and consequently with differ-

ences of vegetation type (from oak to beech forests and clear-cut area) (Tab. 3). In the research of [19, 20], altitude was also recorded as a factor limiting the distribution of millipedes and isopods. As previously stated by many authors, including [9, 14], with elevation, declining densities are expected due to decreased temperatures to suboptimal level, unfavorable conditions for larval development, reduced possibility of hibernation at higher altitude and reduced nutrients availability. In fact, not all species can adapt to unfavorable conditions which lead to low abundances at higher altitudes, and for the representatives of Arachnoidea is well known that prefer shadier habitats. The group of earwigs (Dermaptera) was represented by considerably low number of individuals which is probably due to the trapping efficacy of the pitfall method for active and surface dwelling species.

In conclusion, although Belasica Mt. is not very high, significant differences of community structure throughout altitudinal gradient were registered. While relative abundance of arthropods significantly increased with increasing altitude and differences of vegetation type (from oak to beech forest and clear-cut area), arthropod species richness was influenced only by the increasing altitude. Regarding the results of this study, certain arthropod groups could be used as potential bioindicators when analysing altitudinal influence on arthropods ecology and distribution in mountainous ecosystems.

Relative abundance (ind.trap <sup>-1</sup> )	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14
Aranea	1,75	2,83	2,30	3,23	3,45	4,90	4,16	11,82	16,81	13,77	12,01	10,29	8,38	13,94
Blattodea	0,00	0,00	0,04	0,00	0,09	0,04	0,03	0,41	0,16	0,25	0,03	0,04	0,09	0,58
Chilopoda	0,36	0,46	0,41	0,20	0,14	0,16	0,29	0,30	0,39	0,61	0,53	0,40	0,40	0,63
Coleoptera	5,88	7,68	6,81	6,39	2,43	5,58	13,31	9,88	10,89	37,04	23,21	12,29	8,36	9,09
Coleoptera larvae	0,10	0,14	0,30	0,43	0,20	0,01	0,00	0,01	0,01	0,09	0,11	0,03	0,00	0,06
Dermaptera	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
Diplopoda	0,86	0,74	0,76	1,31	0,58	0,24	1,28	1,80	2,28	1,71	3,76	1,09	2,39	8,20
Isopoda	0,91	1,44	2,25	0,94	0,73	0,65	0,51	0,91	0,10	0,26	0,39	0,35	0,08	2,41
Microcoryphia	0,00	0,00	0,93	0,00	0,00	0,04	0,33	0,80	0,28	0,33	0,46	0,15	0,04	0,04
Opiliones	2,05	1,84	2,15	1,84	1,63	0,54	1,39	1,30	0,46	1,50	1,08	1,03	1,36	0,30
Scorpiones	0,55	0,51	1,25	0,44	0,89	0,75	0,88	0,11	0,03	0,00	0,00	0,00	0,00	0,00

Table 2. Annual relative abundance (ind.trap<sup>-1</sup>) of arthropod groups along altitudinal gradient on Belasica Mt.

Relative abundance (ind.trap <sup>-1</sup> )	Querco- Carpinetum orientalis	Orno- Quercetum petraeae	Festuco hetero- phyllae-Fagetum	Calamintho grandiflorae- Fagetum	Clear-cut area
Aranea	2,71	9,42	13,77	10,22	13,94
Blattodea	0,06	0,16	0,25	0,05	0,58
Chilopoda	0,32	0,28	0,61	0,44	0,63
Coleoptera	5,84	9,91	37,04	14,62	9,09
Coleoptera larvae	0,23	0,01	0,09	0,07	0,06
Dermaptera	0,04	0,00	0,00	0,00	0,00
Diplopoda	0,85	1,40	1,71	2,41	8,20
Isopoda	1,25	0,54	0,26	0,27	2,41
Microcoryphia	0,93	0,36	0,33	0,22	0,04
Opiliones	1,90	0,92	1,50	1,15	0,30
Scorpiones	0,73	0,44	0,00	0,00	0,00

**Table 3.** Annual relative abundance (ind.trap<sup>-1</sup>) of arthropod groups in habitats of different vegetation type on Belasica Mt.

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#### ВЛИЈАНИЈА НА НАДМОРСКАТА ВИСОЧИНА И ВЕГЕТАЦИЈАТА ВРЗ АРТРОПОДНАТА ФАУНА НА ПЛАНИНАТА БЕЛАСИЦА (ЈУГОИСТОЧНА МАКЕДОНИЈА)

#### ПОДНАСЛОВ: СТРУКТУРНИ ОДЛИКИ НА ЕПИГЕЈСКАТА МАКРОФАУНА НА ПЛАНИНАТА БЕЛАСИЦА

#### Александра Цветковска-Ѓорѓиевска, Дана Прелиќ, Славчо Христовски, Валентина Славевска-Стаменковиќ, Милица Ристовска

#### Институт за биологија, Природно-математички факултет, Универзитет "Св. Кирил и Методиј", Скопје, Република Македонија

Извршена е анализа на структурните одлики на артроподната фауна по должина на височински градиент на северните делови од планината Беласица. За таа цел беа поставени вкупно 140 почвени замки по должина на трансект на вкупно 14 истражувани локалитети во периодот април-ноември 2010. Беа регистрирани вкупно 6189 единки кои припаѓаат на 122 таксони (99 видови и 23 морфовидови), 62 фамилии, 14 реда и 5 класи. Со најголемо видово разнообразие се издвојува тврдокрилната фауна (Coleoptera - 110 видови), додека најголем удел во вкупната абундантност на артроподите покажаа Coleoptera (44.76 %) и Araneae (32.47 %), по кои следуваат Diplopoda (7.86 %), Opiliones (5.97 %) и Isopoda (3.57 %). Зголемувањето на надморската височина и соодветните промени на вегетациската структура (промената од дабови кон букови шуми) по должина на градиентот, значително влијаат врз зголемувањето на вкупната бројност на артроподната фауна. Највисоки вредности беа евидентирани во локалитетот под доминација на подгорска бука, на надморска височина од 1100 m, а најниски на надморска височина од 587 m, каде доминира шума од благун и бел габер. Беа констатирани сигнификантни разлики во релативната бројност на Aranea, Coleoptera, Diplopoda, Chilopoda, Microcoryphia и Blattodea помеѓу одделните локалитети. Воедно овие групи покажаа сигнификатно повисока бројност во локалитетите под доминација на подгорска и горска бука, на повисока надморска височина. За разлика од нив, релативната абундантност на Scorpiones, Opiliones и Isopoda покажа значително намалување по должина на градиентот и воедно со преод од дабови кон букови шумски хабитати. Во споредба со вкупната бројност на артроподите, промените на вкупното видово разнообразие се резултат единствено на влијанието на надморската височина.

Клучни зборови: епигејски артроподи, Беласица, влијание на надморска височина,` вегетација ПРИЛОЗИ, Одделение за природно-математички и биотехнички науки, МАНУ, том **41**, бр. 1, стр. 13–23 (2020) CONTRIBUTIONS, Section of Natural, Mathematical and Biotechnical Sciences, MASA, Vol. **41**, No. 1, pp. 13–23 (2020)

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Original scientific paper

#### ON CALCULATING ASSERTION PROBABILITIES FOR PROGRAM FAMILIES

#### Aleksandar S. Dimovski

Faculty for Informatics Sciences, Mother Teresa University, Skopje, Republic of Macedonia

e-mail: aleksandar.dimovski@unt.edu.mk

Highly configurable software systems (program families) appear in many application areas and for many reasons. They can produce a potentially large variety of related programs (variants) by selecting suitable configuration options (features) at compile time. Many of those configurable software systems can input and manipulate uncertain data.

In this paper, we present an approach that calculates the assertion probabilities of program families with uncertain input data. First, we use a combination of forward and backward family-based (lifted) analyses based on abstract interpretation in order to infer necessary preconditions for a given assertion to be satisfied/violated in all variants of a program family. We use lifted analyses based on binary decision diagrams (BDDs) and numerical abstract domains (e.g., Polyhedral) that infer numerical invariants in every program location. Second, model counting techniques are exploited to count the number of solutions to the discovered necessary preconditions (given in the form of linear constraints) on input stores. We use those counts to estimate the probability that the target assertion is satisfied/violated in all variants individually. We implement our approach in a prototype tool, and we evaluate it on several interesting C program families.

Key words: Static analysis by abstract interpretation, Model counting, Software Product Lines (program families)

#### INTRODUCTION

Customization becomes increasingly popular in today's software systems. Many software systems adopt Software Product Line (SPL) methodology [1]. where *features* (statically configured options) are used to control presence and absence of software functionality in a program family. Different family members, called variants or valid products, are derived by switching features on and off, while reuse of the common code is maximized. In fact, the main benefits from using Software Product Lines are: productivity gains, shorter time to market, greater market coverage, etc. Software Product Lines (program families) are commonly seen in development of commercial embedded software, such as in cars, phones, avionics, medicine, robotics, etc. In this case, variation points are used to either support different application scenarios for embedded components, to provide portability across different hardware platforms and configurations, or to

produce variations of products for different market segments or different customers. We consider here SPLs implemented using **#ifdef** directives from the C preprocessor [2]. Many of the above configurable software systems use and manipulate uncertain data. Uncertainty is a common aspect especially for systems that manipulate error-prone data coming from sensors and other external environments. In this case, it is essential to learn how the presence of uncertainty in the input affect the behavior of all valid variants in the family individually.

Probabilistic program analysis [3–5] aims to quantify the probability that a given program satisfies a required property. It has many potential applications, from program understanding and debugging to computing program reliability, compiler optimizations and quantitative information flow analysis for security. In these situations, it is usually more relevant to quantify the probability of satisfying/violating a given property than to just assess the possibility of such events to occur. In this work, we describe an efficient method for probabilistic static analysis of program families. In particular, we show how to calculate the assertion probability, and so estimate the program reliability of all variants, by using static analysis based on abstract interpretation and model counting.

Abstract interpretation [6, 7] is a unifying theory of sound approximation of structures. It represents a well-established general framework, which provides safe and efficient static analyses of real programs. Still, static analysis of program families is harder than static analysis of single programs, because the number of possible variants can be very large (often huge). Therefore, we use so-called family-based (lifted) static analysis [8–10] which works on the family level, analyzing all variants of the family simultaneously at once, without generating any of them explicitly. In particular, we consider here a lifted analysis based on a binary decision diagram (BDD) lifted domain [10], where (Boolean) features are organized in decision nodes and leaf nodes contain a particular analysis property. Elements from the BDD domain are used to map the values of Boolean features (represented in decision nodes) to an analysis property (represented in leaf nodes) for the variant specified by the values of features along the path leading to the leave. The efficiency of BDDs comes from the opportunity to share equal subtrees, in case some properties are independent from the value of some features.

The practical success of abstract interpretation is mainly enabled by the design of numerical abstract domains, which reason on numerical properties of program variables. For example, the polyhedral abstract domain [11] infers linear constraints between all program variables in the form:  $\alpha_1 x_1 + \cdots + \alpha_n x_n + \cdots + \alpha_n + \cdots + \alpha_n x_n + \cdots$  $\alpha_k x_k \ge \beta$ , where  $\alpha_1, \dots, \alpha_k, \beta \in \mathbb{R}$  (reals), and  $x_1, \ldots, x_k$  are program variables. In our case, we use the BDD-based lifted analysis domain, in which the polyhedral domain is used for the leaf nodes. We design two types of static lifted analyses of C program families: a forward analysis to automatically infer invariants in all program locations, and a backward analysis to automatically infer necessary preconditions in all program locations. We combine these two analyses to automatically generate the necessary preconditions on input variables that lead to the satisfaction/violation of a given assertion in a program family. If obtained preconditions are satisfied by some concrete values for input variables, then they represent input values that will allow the given assertion to be satisfied/violated. In fact, we run two backward analyses: the first one determines necessary preconditions for the given assertion to be satisfied, while the second one determines necessary preconditions

for the assertion to be violated.

Model counting is the problem of determining the number of solutions of a given constraint (formula). The LATTE tool [12] implements state-ofthe-art algorithms for computing volumes, both real and integral, of convex polytopes as well as integrating functions over those polytopes. More specifically, we use the LATTE tool and model counting techniques to estimate algorithmically the exact number of points of a bounded (possibly very large) discrete domain that satisfy given linear constraints.

In this work, we describe a method which uses abstract interpretation-based lifted static analysis and model counting to perform a specific type of quantitative analysis of program families, which is the calculation of assertion probabilities. Calculating the probability of a given target assertion involves counting the number of solutions to necessary preconditions that ensure satisfaction/violation of the given assertion for any variant by using model counting, and dividing it by the total space of values of the inputs. We assume that the input values are all uniformly distributed within their finite discrete domain. As the set of obtained necessary preconditions represents an over-approximation of the set of exact input values which guarantee that all executions starting from them lead to satisfaction/violation of the given assertion, we calculate upper and lower bounds of exact probabilities that a given assertion is satisfied or violated. The reported uncertainty is due to the approximation inherent in abstract interpretation, which is introduced in order to obtain a scalable and fully automatic analysis.

We have developed a prototype probabilistic lifted analyzer which uses the BDDAPRON library [13] to implement the BDD lifted domain and the LATTE tool [11] to implement model counting algorithms. BDDAPRON uses the polyhedral numerical domain [11] from the APRON library [14] for the leaf nodes. APRON provides a common high-level API to the most common numerical property domains, such as intervals, octagons, and polyhedral. We have implemented a combination of forward and backward lifted analyses of #ifdef-enriched C programs for the automatic inference of invariants and necessary preconditions in all program locations. In this way, we can use the probabilistic lifted analyzer to calculate assertion probabilities of C program families, which represent majority of industrial embedded code. We restrict our attention on program families that have finite input domains and on polyhedral numerical elements expressed as *linear integer arithmetic* (LIA) constraints over variables whose values are uniformly *distributed* over their assigned interval domains.

The following contributions are made in this work:

- We employ the lifted analysis based on BDDs introduced in [10] and model counting [12] to calculate assertion probabilities in all variants of a program family.
- We provide step-by-step example-driven demonstration of how our approach works.
- We implement our approach using the polyhedral numerical domain from the BDDAPRON library [13] and the LATTE model counting tool [12].
- We evaluate our approach for calculating assertion probabilities on a several interesting #ifdefenriched C programs.

#### MOTIVATING EXAMPLE

To better illustrate the issues we are addressing in this work, we now present a motivating example based on the following program family P:

```
void main() {
       int j := [0,9];
1:
       int i := 0;
linput:
3:
       while (i < 100)
4:
                i := i+1:
5:
                #ifdef(A) j := j+1; #endif
6:
                #ifdef(B) i := i+1; #endif
7:
        ł
l_{final}: assert(j<=105); }
```

The set of Boolean features in the above program family P is  $\mathbb{F} = \{A, B\}$  and the set of configurations is  $\mathbb{K} = \{A \land B, A \land \neg B, \neg A \land B, \neg A \land \neg B\}.$ The family P contains two #ifdef directives, which increase the variable j by 1, depending on which features from  $\mathbb{F}$  are enabled. For each configuration from K a different variant (single program) can be generated by appropriately resolving #ifdef-s. For example, the variant corresponding to the configuration  $A \wedge B$  will have both features A and B enabled (set to true), so that both assignments j := j+1 in program locations 5 and 6 will be included in this variant. On the other hand, the variant for configuration  $\neg A \land \neg B$  will have both features A and B disabled (set to false), so the above assignments in program locations 5 and 6 will not be included in it. There are  $|\mathbb{K}| = 4$  variants in total.

We assume that the initial value of variable j ranges over the integer domain [0, 9], and the chosen initial random value is independently and uniformly distributed across this range. We perform two lifted analyses: a forward invariant and a backward necessary condition, using the BDD lifted domain and the polyhedral numerical domain for the leaf nodes. The forward invariant lifted analysis will find that at the location  $l_{final}$  the following invariants hold (see also the result in Fig. 1a): the invariant ( $200 \le j \le 209$ ) for

the variant  $A \wedge B$ , the invariant (100  $\leq j \leq$  109) for variants  $A \wedge \neg B$  and  $\neg A \wedge B$ , and the invariant  $(0 \le j)$  $\leq 9$ ) for the variant  $\neg A \land \neg B$ . Therefore, the target assertion ( $j \le 105$ ) is always violated for the variant  $A \wedge B$  and it is always satisfied for the variant  $\neg A \wedge$  $\neg B$ . However, for variants  $A \land \neg B$  and  $\neg A \land B$ , the assertion can be both satisfied and violated. In those cases, we perform a backward necessary condition lifted analysis for assertion satisfaction/violation, which computes the preconditions on input states such that all executions starting from those states will satisfy/violate the given assertion. The backward necessary condition analysis for variants  $A \wedge \neg B$  and  $\neg A \land B$  will infer the precondition  $(0 \le j \le 5)$  at location *l<sub>input</sub>* for the assertion to be satisfied, while the precondition ( $6 \le j \le 9$ ) at location  $l_{input}$  will be inferred for the assertion to be violated (see the results in Fig. 1b and 1c). The size of the input domain is 10, since j belongs to [0, 9]. By calling the LATTE tool to count the number of solutions to the above preconditions, we can calculate that the probability for the assertion to be satisfied (success probability) is less or equal to: 0=0% for the variant  $A \wedge B$ , 6/10=60% for variants  $A \wedge \neg B$  and  $\neg A \wedge B$ , and 1=100% for the variant  $\neg A \land \neg B$ . On the other hand, the probability for the assertion to be violated (*failure probability*) is less or equal to: 1=100% for the variant  $A \wedge B$ , 4/10=40% for variants  $A \wedge \neg B$  and  $\neg A \wedge B$ , and 0=0% for the variant  $\neg A \land \neg B$ .

Fig. 1 shows the analysis results given as BDDs obtained using the forward invariant analysis and two backward necessary condition analysis for assertion satisfaction and violation. Note that the inner nodes of BDDs in Fig. 1 are labelled with features from  $\mathbb{F}$ , the leaves are labelled with the elements from the polyhedral domain, and the edges are labeled with the truth value of the decision on the parent node, true or false (we use solid edges for true, and dashed edges for false). We can see that BDDs offer possibilities for sharing and interaction between analysis properties corresponding to different variants. Thus, they provide symbolic and compact representation of lifted analysis elements. For example, the cases when (A is true and *B* is false) and (*A* is false and *B* is true) are identical, so they share the same leaf nodes in all three BDDs in Fig. 1. Notice that, in the worst case, BDDs still need K different leaf nodes, but experimental evidence shows that sharing often occurs in practice.

#### PROGRAMMING LANGUAGE

Let  $\mathbb{F} = \{A1, ..., An\}$  be a finite and totally ordered set of Boolean variables representing the *features* available in a program family. The total ordering of features is:  $A1 < \cdots < An$ . A specific subset of features,  $k \subseteq \mathbb{F}$ , known as *configuration*, specifies a variant (valid product) of a program family. We assume that only a subset  $\mathbb{K} \subseteq 2^{\mathbb{F}}$  of all possible configurations are *valid*. An alternative representation of configurations is based upon propositional formulae. Each configuration  $k \in \mathbb{K}$  can be represented by a formula:  $k(A1) \land ... \land k(An)$ , where k(Ai) = Ai if  $Ai \in k$ , and  $k(Ai) = \neg Ai$  if  $Ai \notin k$  for  $1 \le i \le n$ . We will use both representations interchangeably.

We define *feature expressions*, denoted FeatExp( $\mathbb{F}$ ), as the set of well-formed propositional logic formulae over  $\mathbb{F}$  generated by the grammar:

$$\theta ::= true \mid A \in \mathbb{F} \mid \neg \theta \mid \theta \land \theta$$

We will use  $\theta \in \text{FeatExp}(\mathbb{F})$  to define presence conditions in program families.

We consider a programming language that is a subset of C for writing program families, which will be used to exemplify our work. The language is extended with a compile-time conditional statement for encoding multiple variants of a program. The new statement ``#ifdef ( $\theta$ ) s'' contains a feature expression  $\theta \in \text{FeatExp}(\mathbb{F})$  as a presence condition, such that only if  $\theta$  is satisfied by a configuration  $k \in$ K then the statement s will be included in the variant



**Fig. 1.** BDD-based lifted analyses results obtained using a forward invariant analysis and two backward necessary condition analyses for assertion satisfaction and violation. We use solid edges for true, and dashed edges for false.

corresponding to k. The syntax of the language is:

$$\begin{split} s ::= & \text{skip} | x := e | x := [n,n'] | s1; s2 | \text{if } (e) \text{ then } s1 \text{ else } s2 \\ | \text{ while } (e) \text{ do } s | \text{ \#ifdef } (e) s | \text{ assert } (e) \\ e ::= n | x | e1 \oplus e2 \end{split}$$

where n ranges over integers, [n, n'] ranges over integer intervals, x ranges over variable names Var, and ⊕ over binary arithmetic-logic operators. Non-deterministic interval assignment x := [n, n'] represents an input statement which assigns to the input variable x an uniformly distributed random integer from the interval [n, n']. The interval assignment can occur only in the input section of the program. The set of all generated statements s is denoted by Stm, whereas the set of all expressions e is denoted by Exp. We assume *linput* is the location after the input statements (i.e. it denotes the end of input section) and lfinal is the location at the end of the program, where an assertion assert(e<sub>f</sub>) is posed. Without loss of generality, a program is a sequence of statements followed by a single assertion.

The program families are evaluated in two stages. First, a preprocessor takes as input a program family and a configuration  $k \in \mathbb{K}$ , and outputs a var-

iant, i.e. a single program without #ifdef-s, corresponding to k. Second, the obtained variant is evaluated using the standard single-program semantics [14]. The first stage is specified by the projection function  $\mathcal{P}_k$ , which is an identity for all basic statements of the program family and recursively pre-processes all sub-statements of compound statements. Hence,  $\mathcal{P}_k(\text{skip}) = \text{skip}$  and  $\mathcal{P}_k(s; s') = \mathcal{P}_k(s)$ ;  $\mathcal{P}_k(s')$ . The interesting case is ``#ifdef ( $\theta$ ) s'' statement, where the statement s is included in the resulting variant iff k satisfies  $\theta$ , otherwise the statement s is removed (i.e. replaced with Skip). Thus,

> $\mathcal{P}_k(\text{#ifdef }(\theta) \text{ s}) = \mathcal{P}_k(\text{s}), \text{ if } k \text{ satisfies } \theta, \text{ and}$  $\mathcal{P}_k(\text{#ifdef }(\theta) \text{ s}) = \text{skip, if } k \text{ does not satisfy } \theta$

#### SINGLE-PROGRAM STATIC ANALYSES

In this section, we introduce the combination of forward and backward single-program analyses for inferring necessary preconditions that a given assertion is satisfied/violated. Those preconditions are used for computing the probabilities that the given assertion is satisfied (called *success probability*) or violated (called *failure probability*). For easy presentation, we focus on single programs in this section, and then show how to extend our technique to program families in the next section. We introduce basic theoretical concepts only as required.

Recall the running example program family P from "Motivating example" section. The variant corresponding to the configuration  $A \land \neg B$  is:

1: int j := [0,9];int i := 0; linput: while (i<100) { 3: 4: i := i+1;5: j := j+1; 6: skip; 7: } assert(j<=105); l<sub>final</sub>: We denote it as  $\mathcal{P}_{A \wedge \neg B}(\mathbf{P})$ .

**Concrete semantics**. The "*state*" of an imperative program is a program control location, together with the values of all variables in that location. The semantics of a single program is given by defining a state transition function *trans*, as follows:

 $State = Program \ location \times Store$  $Store = Variables \rightarrow Value$  $trans : State \rightarrow State$ 

We first introduce a *collecting (concrete) se-mantics* which associates with each program location the set of all memory stores that can ever occur when program control reaches that location. We assume the program is run on data from a set  $\mathbb{E} \in 2^{Store}$  of possible initial input stores. Let  $l_{input}$  be the program's input location and let l be another program point. The set of stores that can be reached at location l are defined:

 $coll_l = \{s \mid (l,s) = trans^n (l_{input}, s_0), s_0 \in \mathbb{E}, n \ge 0\}$ where  $trans^n$  is the n-th iterate of trans (i.e.  $trans^n = trans \circ trans^{n-1}$ ). The collecting semantics thus associates with each program location the set of stores  $coll_l \in 2^{Store}$ .

For the running example  $\mathcal{P}_{A \wedge \neg B}(\mathbf{P})$ , there are two variables i and j. Thus, a set of stores has the form:

 $\{[i \mapsto v_1, j \mapsto n_1], [i \mapsto v_2, j \mapsto n_2] \dots\}$ 

where  $[i \mapsto v_1, j \mapsto n_1], [i \mapsto v_2, j \mapsto n_2] \in Store$ . For notational simplicity, we can identify this set with the set:

{[i  $\mapsto$  { $v_1$ ,  $v_2$ , ... }, j  $\mapsto$  { $n_1$ ,  $n_2$ , ... }]} Given an initial input set  $\mathbb{E} =$  {[j  $\mapsto$  {0, ...,9}]}, the set of stores reachable at all program locations are:

 $\begin{array}{l} coll_3 = \{ [i \mapsto \{0\}, j \mapsto \{0, \dots, 9\}] \} \\ coll_4 = \{ [i \mapsto \{0, \dots, 99\}, j \mapsto \{0, \dots, 108\}] \} \\ coll_5 = \{ [i \mapsto \{1, \dots, 100\}, j \mapsto \{0, \dots, 108\}] \} \\ coll_6 = \{ [i \mapsto \{1, \dots, 100\}, j \mapsto \{0, \dots, 109\}] \} \end{array}$ 

$$coll_7 = \{ [i \mapsto \{1, ..., 100\}, j \mapsto \{0, ..., 109\} ] \}$$
$$coll_{l_{final}} = \{ [i \mapsto \{100\}, j \mapsto \{100, ..., 109\} ] \}$$

The set  $2^{Store}$  of all sets of stores forms a lattice with set inclusion  $\subseteq$  as its partial order, so any two store sets A, B have least upper bound  $A \cup B$  and greatest lower bound  $A \cap B$ . The lattice  $2^{Store}$  is complete, meaning that any collection of sets of stores has a least upper bound in  $2^{Store}$ , namely its union. The above sets of reachable stores  $coll_l$  can be obtained as *solution* to the following *forward data-flow equations*, which have a unique least fixpoint solution by completeness of  $2^{Store}$ .

$$\begin{aligned} & coll_{input} = \mathbb{E} \\ & coll_3 = coll_{input} \cap \{[i \mapsto \{0\}, j \mapsto \mathbb{N}]\} \\ & coll_4 = (coll_3 \cup coll_7) \cap \{i \mapsto \{0, \dots, 99\}, j \mapsto \mathbb{N}\} \\ & coll_5 = \{[i \mapsto v + 1, j \mapsto coll_4(j)] | v \in coll_4(i)\} \\ & coll_6 = \{[i \mapsto coll_5(i), j \mapsto n + 1)] | n \in coll_5(j)\} \\ & coll_7 = coll_6 \\ & coll_{lfinal} = (coll_3 \cup coll_7) \cap \{[i \mapsto \{100, \dots\}, j \mapsto \mathbb{N}]\} \end{aligned}$$

where  $coll_l(j)$  denotes the set of values assigned to the variable j at location *l*. From the solution of the above equations for  $coll_{l_{final}}(j) = \{100, ..., 109\}$ , we can see that the target assertion ( $j \le 105$ ) can be both satisfied and violated for the variant  $A \land \neg B$ .

In order to determine the success and failure probabilities for the variant  $A \land \neg B$ , we need to calculate a backward collecting semantics, which given a set of final stores finds at each program location the set of stores necessary to imply the given set of final stores at termination. For the running example program, the appropriate backward data-flow equations are:

$$\begin{split} b\_coll_{linput} &= \{ [j \mapsto b\_coll_3(j)] \mid 0 \in b\_coll_3(i) \} \\ b\_coll_3 &= (b\_coll_{lfinal} \cap \{ [i \mapsto \{100, \dots\}, j \mapsto \mathbb{N}] \} \} \cup (b\_coll_4 \cap \{ [i \mapsto \{0, \dots, 99\}, j \mapsto \mathbb{N}] \} ) \\ b\_coll_4 &= \{ [i \mapsto v, j \mapsto b\_coll_5(j)] | v + 1 \in b\_coll_5(i) \} \end{split}$$

$$b_{coll_{5}} = \{ [i \mapsto b_{coll_{6}}(i), j \mapsto n] | n + 1 \in b_{coll_{6}}(j) \}$$

$$\begin{split} b\_coll_6 &= b\_coll_7 \\ b\_coll_7 &= (b\_coll_{final} \cap \{[i \mapsto \{100, \dots\}, j \mapsto \mathbb{N}]\}) \cup (b\_coll_4 \cap \{[i \mapsto \{100, \dots\}, j \mapsto \mathbb{N}]\}) \end{split}$$

where  $b_ccoll_l$  is the set of all stores at location l that cause control to reach point  $l_{final}$  with a final store  $b_ccoll_{l_{final}}$ . Note that,  $b_ccoll_{l_{final}}$  is a parameter for the above equation system. Now, we find solutions of two backward data-flow equations: the first one when  $b_ccoll_{l_{final}} = \{[i \mapsto \mathbb{N}, j \mapsto \{100, \dots, 105\}]\}$  which

causes the target assertion to be satisfied; and the second one when  $b_ccoll_{l_{final}} = \{[i \mapsto \mathbb{N}, j \mapsto \{106, ..., 109\}]\}$  which causes the target assertion to be violated. From the solution of the first backward equations, we obtain  $b_ccoll_{l_{input}}(j) = \{0, 1, 2, 3, 4, 5\}$ , that is  $\mathbb{E}_{sat} = [j \mapsto \{0, 1, 2, 3, 4, 5\}]$ . From the solution of the second backward equations, we obtain  $b_ccoll_{l_{input}}(j) = \{6, 7, 8, 9\}$ , that is  $\mathbb{E}_{viol} = [j \mapsto \{6, 7, 8, 9\}]$ . Therefore, we conclude that the success probability is  $Pr^s(\mathcal{P}_{A \wedge \neg B}(P)) = \frac{|\mathbb{E}_{sat}|}{|\mathbb{E}|} = \frac{6}{10} = 60\%$ and the failure probability is  $Pr^f(\mathcal{P}_{A \wedge \neg B}(P)) = \frac{|\mathbb{E}_{viol}|}{|\mathbb{E}|} = \frac{4}{10} = 40\%$ .

Abstract semantics. The collecting concrete semantics is obviously *incomputable*, due to the insolvability of the halting problem and nearly any other question concerning program behavior. Therefore, we seek for sound approximations. We demonstrate how to derive approximate, but computable analyses, which statically determine dynamic properties of programs. The effect of thus obtained abstract analyses is that the price paid for finite computability is loss of precision. The abstract analyses will infer necessary preconditions on input stores so that all executions starting from those input stores lead to satisfaction (resp., violation) of the final assertion. In this way, we will compute the over-approximations of sets  $\mathbb{E}_{sat}$  and  $\mathbb{E}_{viol}$ , and thus find the lower and upper bounds for  $Pr^s$  and  $Pr^f$ .

Recall that the collecting semantics works on sets of stores,  $2^{Store}$ . Various approximations can be expressed by simpler domains (lattices) *Abs*, connected to  $2^{Store}$  by an abstraction function  $\alpha: 2^{Store} \rightarrow Abs$ , and a dual concretization function  $\gamma: Abs \rightarrow 2^{Store}$ . Here, *Abs* represents a lattice of approximate descriptions of sets of stores  $2^{Store}$ . The pair of functions  $\alpha$  and  $\gamma$ , which capture information loss between two domains (lattices)  $2^{Store}$  and *Abs*, are required to form a Galois connection [6, 15]. Abstract analysis may thus be thought of as executing the program over a lattice of imprecise but computable abstract store descriptions instead of the precise and incomputable collecting semantics lattice.

There exist various abstract domains, which can be used for automatic discovery of program properties. They differ in expressive power and computational complexity. The most suitable abstract domain for computing necessary preconditions on input stores is the polyhedral numerical domain [11]. The polyhedral domain is a fully relational numerical property domain, which allows manipulating conjunctions of linear inequalities of the form  $\alpha_1 x_1 + \beta_1 = 0$ 

 $\dots + \alpha_k x_k \ge \beta$ , where  $\alpha_1, \dots, \alpha_k, \beta \in \mathbb{R}$  (reals), and  $x_1, \dots, x_k$  are program variables. Polyhedral analysis is computationally expensive but very precise.

The polyhedral abstract domain  $\mathbb{P}$  is equipped with (over-approximating) sound operators for abstraction  $\alpha_{\mathbb{P}}: 2^{Store} \to \mathbb{P}$ , concretization  $\gamma_{\mathbb{P}}: \mathbb{P} \to$  $2^{Store}$ , partial ordering  $\sqsubseteq_{\mathbb{P}}$ , least upper bound (join)  $\sqcup_{\mathbb{P}}$ , greatest lower bound (meet)  $\sqcap_{\mathbb{P}}$ , the least element (bottom)  $\perp_{\mathbb{P}}$ , the greatest element (top)  $I_{\mathbb{P}}$ , as well as sound transfer functions for assignments  $assign_{\mathbb{P}}: Stm \times \mathbb{P} \to \mathbb{P}$ , tests (which occur in whiles and if-s)  $filter_{\mathbb{P}}: Exp \times \mathbb{P} \to \mathbb{P}$ , backward assignments  $b_{assign_{\mathbb{P}}}$ :  $Stm \times \mathbb{P} \to \mathbb{P}$ , and backward tests  $b_{filter_{\mathbb{P}}}: Exp \times \mathbb{P} \to \mathbb{P}$ . For example, the transfer function  $filter_{\mathbb{P}}(e,p)$  returns an abstract store p'which is restriction of the abstract store p, so that it satisfies the given test (expression) e. The domain  $\mathbb{P}$ also contains widening  $\Delta_{\mathbb{P}}$  and narrowing  $\bigcirc_{\mathbb{P}}$  operators in order to compute an over-approximation of least fixpoints.

We define a system of *approximate (abstract)* forward data-flow equations, which describe the program's behavior on  $Abs = \mathbb{P}$ . We model concrete data-flow equations by applying the abstraction function  $\alpha_{\mathbb{P}}: 2^{Store} \longrightarrow \mathbb{P}$  to the sets involved in equations. Set inclusion  $\subseteq$ , union  $\cup$ , and intersection  $\cap$  in the world of actual, concrete computations are modeled by  $\sqsubseteq_{\mathbb{P}}, \sqcup_{\mathbb{P}}$ , and  $\sqcap_{\mathbb{P}}$  in the world of abstract computations over  $\mathbb{P}$ . Thus, we obtain the following system of abstract forward data-flow equations:

$$inv_{linput} = \alpha_{\mathbb{P}}(\mathbb{E})$$

$$inv_{3} = assign_{\mathbb{P}}(i \coloneqq 0, inv_{linput})$$

$$inv_{4} = (inv_{3} \sqcup_{\mathbb{P}} inv_{7}) \sqcap_{\mathbb{P}} filter_{\mathbb{P}}(i < 100, \mathbb{I}_{\mathbb{P}})$$

$$inv_{5} = assign_{\mathbb{P}}(i \coloneqq i + 1, inv_{4})$$

$$inv_{6} = assign_{\mathbb{P}}(j \coloneqq j + 1, inv_{5})$$

$$inv_{7} = inv_{6}$$

$$inv_{l_{final}} = (inv_{3} \sqcup_{\mathbb{P}} inv_{7}) \sqcap_{\mathbb{P}} filter_{\mathbb{P}}(\neg(i < 100), \mathbb{I}_{\mathbb{P}})$$

The lattice  $\mathbb{P}$  is also complete, so the above equation system has a unique least fixpoint solution. The two forward data-flow equation systems, *coll* and *inv*, are related by:  $inv_l \supseteq_{\mathbb{P}} \alpha_{\mathbb{P}}(coll_l)$  for any program location *l*. This is the *soundness* relation showing that stores computed by abstract equations  $inv_l$  over-approximate the stores computed by concrete equations  $coll_l$ , for any location *l*. For the running example  $\mathcal{P}_{A \wedge \neg B}(\mathbb{P})$ , we obtain the following solution for  $inv_{l_{final}} = (100 \le j \le 109)$ . Hence, we conclude that the assertion at  $l_{final}$  can be satisfied for  $p_{final}^{sat} = filter_{\mathbb{P}} (j \le 105, inv_{l_{final}}) = (100 \le j \le 105)$ , and the assertion at  $l_{final}$  can be violated for

 $p_{final}^{viol} = filter_{\mathbb{P}} \left( \neg (j \le 105), inv_{l_{final}} \right) = (106 \le j \le 109).$ 

We now design two abstract backward interpreters that propagate backwards the invariants ensuring that the final assertion is satisfied  $p_{final}^{sat}$  and violated  $p_{final}^{viol}$ , respectively. The abstract backward interpreters refine the invariants found by *inv*. We have the following system of abstract backward data-flow equations:

$$cond_{linput} = b\_assign_{\mathbb{P}}(i \coloneqq 0, cond_{3})$$
  

$$cond_{3} = (cond_{l_{final}} \sqcap_{\mathbb{P}} b\_filter_{\mathbb{P}}(\neg(i < 100, I_{\mathbb{P}})) \sqcup_{\mathbb{P}} (cond_{4} \sqcap_{\mathbb{P}} b\_filter_{\mathbb{P}}(i < 100, I_{\mathbb{P}}))$$
  

$$cond_{4} = b\_assign_{\mathbb{P}}(i \coloneqq i + 1, cond_{5})$$
  

$$cond_{5} = b\_assign_{\mathbb{P}}(j \coloneqq j + 1, cond_{6})$$
  

$$cond_{6} = cond_{7}$$
  

$$cond_{7} = (cond_{l_{final}} \sqcap_{\mathbb{P}} b\_filter_{\mathbb{P}}(\neg(i < 100, I_{\mathbb{P}})))$$
  

$$\sqcup_{\mathbb{P}} (cond_{4} \sqcap_{\mathbb{P}} b\_filter_{\mathbb{P}}(i < 100, I_{\mathbb{P}}))$$

The solution of the above system when  $cond_{l_{final}} = p_{final}^{sat}$  is  $cond_{l_{input}}^{sat} = (0 \le j \le 5)$ , whereas when  $cond_{l_{final}} = p_{final}^{viol}$  is  $cond_{l_{input}}^{viol} = (6 \le j \le 9)$ . Next, we call the LATTE tool to count the number of solutions from the input domain  $j \in [0,9]$  to the above preconditions  $cond_{l_{input}}^{sat}$  and  $cond_{l_{input}}^{viol}$ . Finally, we obtain that the success probability is  $Pr^{s}(\mathcal{P}_{A \land \neg B}(P)) = 60\%$  and  $Pr^{f}(\mathcal{P}_{A \land \neg B}(P)) = 40\%$ . Note that, for this running example the abstract analyses do not lose any precision, and they compute the same results for the success and failure probabilities as the concrete semantics. However, in general it is possible to lose some precision by abstract analyses, so the computed results represent lower and upper bounds of the exact ones. We now show one example, where we obtain approximate results. Consider the following program P':

void main() {

1: int x := [0,9], y:=[0,9]; *l<sub>input</sub>*: int s := x - y; 3: if (s>=2) y:=y+2; *l<sub>final</sub>*: assert (y>3); }

The forward analysis will infer that the program can both satisfy and violate the assertion. The backward necessary condition analysis for assertion satisfaction will discover the constraint:  $x + 2y \ge$  $8 \land 0 \le x \le 9 \land 2 \le y \le 9$ , thus we find that the upper bound probability for assertion satisfaction is 74%. Moreover, the input stores that do not satisfy the above precondition definitely lead to the assertion violation. Thus, the lower bound probability for assertion violation is 100%-74%=26%. The backward necessary precondition analysis for assertion violation will discover the constraint:  $x + 5y \le 23 \land 0 \le x \le 9 \land 0 \le y \le 3$ , thus we find that the upper bound probability for assertion violation is 32 %. By similar reasoning as above, the lower bound probability for assertion satisfaction is 68 %. On the other hand, we can calculate by hand that the success probability is exactly 71 %, while the failure probability is exactly 29 %.

#### FAMILY-BASED (LIFTED) STATIC ANALYSES

Lifted analyses are designed by *lifting* existing single-program analyses to work on program families, rather than on individual programs. They directly analyze the code base of program families, without preprocessing them by taking the variability introduced by **#ifdef-s** into account.

**Concrete semantics**. Since, we work with program families, we lift all definitions for single-program analyses configuration-wise. Thus, we work with *lifted stores*  $\overline{Store} = Store^{\mathbb{K}} = \prod_{k \in \mathbb{K}} Store$  and *lifted states*  $\overline{State} = State^{\mathbb{K}} = \prod_{k \in \mathbb{K}} State$ , which represent a tuple of  $|\mathbb{K}|$  copies of Store and State, one for each valid configuration. Given a lifted store  $\overline{s} \in \overline{State}, \pi_k(\overline{s})$  selects the k-th component of the tuple  $\overline{s}$ . We also work with a *lifted transition function*  $\overline{trans}: (State \to State)^{\mathbb{K}}$ , which represents a tuple of  $|\mathbb{K}|$  independent simple functions, for which the k-th component of the function value only depends on the k-th component of the argument.

The collecting lifted semantics works on lifted stores and defines the set of lifted stores that can be reached at some program location *l*:

$$\overline{coll}_{l} = \{ \overline{s} \mid (l, \overline{s}) = \overline{trans}^{n} (l_{input}, \overline{s_{0}}), \overline{s_{0}} \in \overline{\mathbb{E}}, n \ge 0 \}$$

where  $\overline{\mathbb{E}} \in 2^{\overline{Store}}$  is the set of input lifted stores. We now show how our approach works for the running example family P from "Motivating example" section. The program family P has two variables i and j, and four configurations  $\mathbb{K} = \{A \land B, A \land \neg B, \neg A \land B, \neg A \land \neg B\}$ . The set of input lifted stores is  $\overline{\mathbb{E}} = \{([j \mapsto \{0, ..., 9\}], [j \mapsto \{0, ..., 9\}], [j \mapsto \{0, ..., 9\}], [j \mapsto \{0, ..., 9\}]\}$  for  $\overline{\mathbb{E}} = \{\prod_{k \in \mathbb{K}} [j \mapsto \{0, ..., 9\}]\}$  for short. The first component of a lifted store, i.e. a tuple,  $([j \mapsto 0], [j \mapsto 0], [j \mapsto 0], [j \mapsto 0], [j \mapsto 0]\}$  corresponds to config.  $A \land B$ , the second to  $A \land \neg B$ , the third to  $\neg A \land B$ , and the fourth to  $\neg A \land \neg B$ . Forward and backward concrete lifted data-flow equations are the same as for single programs, except that they now work on lifted stores instead of stores. For example, we have:

$$\overline{coll}_{l_{innut}} = \overline{\mathbb{E}}$$

20

$$\begin{split} \overline{coll_3} &= \overline{coll}_{l_{input}} \overline{\cap} \{ \prod_{k \in \mathbb{K}} [i \mapsto \{0\}, j \mapsto \mathbb{N}] \} \\ \overline{b\_coll}_{l_{input}} &= \{ \prod_{k \in \mathbb{K}} [j \mapsto \pi_k(\overline{b_{coll_3}}(j))] \mid 0 \in \\ \overline{\pi_k(b_{coll_3}}(i)) \} \end{split}$$

where  $\overline{\cap}$ ,  $\overline{\cup}$  are lifted versions of intersection and union that work on tuples. We obtain the following solution for the above forward lifted equations  $\overline{coll_{final}} = \{ ([i \mapsto \{100\}, j \mapsto \{200, \dots, 209\}], [i \mapsto \{100\}, j \mapsto \{200, \dots, 209\} \} \}$  $\{100\}, j \mapsto \{100, \dots, 109\}$ ,  $[i \mapsto \{100\}, j \mapsto$  $\{100, ..., 109\}$ ,  $[i \mapsto \{100\}, j \mapsto \{0, ..., 9\}]$ ). We can see that the target assertion ( $j \le 105$ ) is definitely violated for  $A \wedge B$ , and satisfied for  $\neg A \wedge \neg B$ . Therefore, the success probability  $Pr^s$  that a variant satisfies the tarassertion is:  $Pr^{s}(\pi_{A \wedge B}(P)) = 0\%$ get and  $Pr^{s}(\pi_{\neg A \land \neg B}(P)) = 100\%$ , whereas the failure probability  $Pr^{f}$  that a variant violates a target asser- $Pr^f(\pi_{A \wedge B}(P)) = 100\%$ is: tion  $Pr^f(\pi_{\neg A \land \neg B}(P)) = 0\%$ . In order to determine the success and failure probabilities for variants  $A \wedge \neg B$ and  $\neg A \land B$ , we run two backward collecting lifted semantics: one for assertion satisfaction and one for assertion violation. Similarly as in the previous section, we can establish that  $Pr^{s}(\mathcal{P}_{A\wedge\neg B}(\mathbf{P})) =$ 

 $Pr^{s}(\mathcal{P}_{\neg A \land B}(\mathbf{P})) = 60\%$  and  $Pr^{f}(\mathcal{P}_{A \land \neg B}(\mathbf{P})) =$ 

**Abstract semantics**. Polyhedral abstract lifted analyses work on lifted domain  $\overline{\mathbb{P}} = \mathbb{P}^{\mathbb{K}} = \prod_{k \in \mathbb{K}} \mathbb{P}$ , which contains one separate copy for each configura-

tion of  $\mathbb{K}$ . All abstract operations that work for  $\mathbb{P}$  are

lifted configuration-wise to work for  $\mathbb{P}^{\mathbb{K}}$ . Thus, we

 $Pr^f(\mathcal{P}_{\neg A \land B}(\mathbf{P})) = 40\%.$ 

have lifted versions of partial ordering  $\doteq$ , join  $\dot{\sqcup}$ , meet  $\dot{\sqcap}$ , bottom  $\dot{\bot} = (\bot_{\mathbb{P}}, ..., \bot_{\mathbb{P}})$ , top  $\dot{\uparrow} = (\mathsf{T}_{\mathbb{P}}, ..., \mathsf{T}_{\mathbb{P}})$ , widening  $\dot{\Delta}$ , and narrowing  $\dot{\odot}$ . There are also lifted versions of transfer functions for assignments  $\overline{assign}_{\mathbb{P}}: Stm \times \mathbb{P} \to \mathbb{P}$ , tests  $\overline{filter}_{\mathbb{P}}: Exp \times \mathbb{P} \to \mathbb{P}$ , backward assignments  $\overline{b\_assign}_{\mathbb{P}}: Stm \times \mathbb{P} \to \mathbb{P}$ , and backward tests  $\overline{b\_filter}_{\mathbb{P}}: Exp \times \mathbb{P} \to \mathbb{P}$ . Finally, we define two transfer functions to handle variability introduced by ``#ifdef ( $\theta$ ) s'' statements:

$$\overline{f\_filter}(\theta, \bar{p}) = \prod_{k \in \mathbb{K}} \pi_k(\bar{p}), \text{ if } k \text{ satisfies } \theta$$

$$\overline{ifdef}(\#ifdef(\theta) s, \bar{p}) =$$

$$\overline{ifdef}(\#ifdef(\theta) s, \bar{p}) =$$

 $[[\bar{s}]](f\_filter(\theta,\bar{p})) \sqcup f\_filter(\neg\theta,\bar{p})$ 

where  $[[\bar{s}]]$  represents the lifted transfer function for the statement s. The function  $\overline{f_f llter}$  keeps those components k of the input tuple  $\bar{p}$  that satisfy  $\theta$ , and replaces the other components of  $\bar{p}$  with  $\bot_{\mathbb{P}}$ . The function  $\overline{if def}$  captures the effect of analyzing the statement s in those components k of the input tuple  $\bar{p}$  that satisfy  $\theta$ , otherwise it is an identity for the other components of  $\bar{p}$ . Now, if we perform abstract lifted forward and backward analyses for the running example P, we can calculate the exact values for the success and failure probabilities for all four variants. For example, some abstract forward lifted data-flow equations are:

$$\overline{inv}_{6} = \overline{ifdef}(\#if(A) \ j \coloneqq j+1, inv_{5})$$
  
$$\overline{inv}_{7} = \overline{ifdef}(\#if(B) \ j \coloneqq j+1, inv_{6})$$

**Optimization**. We can speed up the abstract lifted analyses by using *shared representation* to represent sets of configurations with equivalent analysis

 Table 1. Experimental evaluation of probabilistic lifted analysis based on BDDs vs. probabilistic lifted analyses based on tuples . All times are in seconds.

Bonch	cource	ITCI	LOC	E	BDD <sup>10</sup>	В	EVACT	
Denen.	source	r	LUC	TIME <sup>10</sup>	IMPROVE <sup>10</sup>	TIME <sup>1000</sup>	IMPROVE <sup>1000</sup>	EAACI
count_up_down*.c	loops	4	25	0.018	5 ×	0.019	$5 \times$	
hhk2008.c	loop-lit	5	25	0.037	8.5 ×	0.040	$9 \times$	
gsv2008.c	loop-lit	2	25	0.006	$2 \times$	0.007	$2 \times$	
bwd_loop2.c	[12]	2	15	0.007	$2.1 \times$	0.007	$2 \times$	
example7.c	[13]	4	20	0.013	6 ×	0.014	6.5 ×	≈

information. For this aim, we use *binary decision diagrams* (BDDs) as lifted analysis domains. We exploit the well-known efficiency of BDDs [16, 17] for representing formulae that combine Boolean variables and analysis properties. The elements of the BDD domain are disjunctions of the leaf nodes that belong to an existing (single-program) analysis do-

main (e.g. the polyhedral domain), which are separated by the values of Boolean features organized in the decision nodes. Therefore, we encapsulate the set  $\mathbb{K}$  into the decision nodes of a BDD where each top-down path represents one or several configurations from  $\mathbb{K}$ , and we store in each leaf node the property generated from the variants derived by the corresponding configurations.

We now formally define the lifted domain of BDDs. A binary decision tree (BDT)  $t \in \mathbb{T}(\mathbb{F}, \mathbb{P})$ over the set of features  $\mathbb{F}$  and the leaf Polyhedral domain  $\mathbb{P}$  is either a leaf  $\langle p \rangle$  with  $p \in \mathbb{P}$  and  $\mathbb{F} = \emptyset$ , or [A:tl,tr] where A is the *smallest element* of  $\mathbb{F}$  with respect to its ordering, *tl* is the left subtree of *t* representing its true branch, and tr is the right subtree of t representing its false branch, such that  $tl, tr \in$  $\mathbb{T}(\mathbb{F}\setminus\{A\},\mathbb{P})$ . Recall that  $\mathbb{F} = \{A1, \dots, An\}$  is a totally ordered set with ordering  $A1 < \cdots < An$ . There are several reductions that can be applied to BDTs in order to remove the redundancy from their representation [16, 17]: Removal of duplicate leaves; Removal of redundant tests; and Removal of duplicate nonleaves. If we apply the above reductions to a BDT t, we obtain a reduced *binary decision diagram* (BDD)  $d \in \mathbb{D}(\mathbb{F}, \mathbb{P})$ . Thanks to the sharing of information enabled by the above reductions, BDDs are quite compact representation of tuples from  $\mathbb{P}^{\mathbb{K}}$ . Moreover, if the ordering on the features from  $\mathbb{F}$ , occurring on any path is fixed, then the resulting BDDs have a canonical form. This means that any property from the lifted domain  $\mathbb{P}^{\mathbb{K}}$  can be represented in a unique way by a BDD.

For example, consider the running example program family P. If we use the lifted analysis domain  $\mathbb{P}^{\mathbb{K}}$ , we obtain the following solutions of abstract lifted analyses.

$$\begin{split} \overline{inv}_{l_{final}} &= \{(200 \le j \le 209, 100 \le j \le 109, 100 \le j \le 109, 0 \le j \le 109, 0 \le j \le 9)\}\\ \hline cond^{sat}_{l_{input}} &= \{(\bot_{\mathbb{P}}, 0 \le j \le 5, 0 \le j \le 5, 0 \le j \le 9)\}\\ \hline cond^{viol}_{l_{input}} &= \{(0 \le j \le 9, 6 \le j \le 9, 6 \le j \le 9, \bot_{\mathbb{P}})\} \end{split}$$

If we use the BDD-based lifted domain instead, the BDDs representing the above locations are given in Figure 1. They use three polyhedral properties instead of four as above in case of tuples. Moreover, for the input lifted store, the tuple-representation is  $\overline{mv}_{l_{input}} = \{(0 \le j \le 9, 0 \le 1, 0 \le$ 

9)}, while the BDD representation uses only one polyhedral property, thus maximizing the effects of sharing. This ability for sharing is the key motivation behind the introduction of the BDD-representation.

#### **EXPERIMENTS**

In this section, we evaluate our approach for computing assertion probabilities of program families. We have implemented a prototype lifted static analyzer for analyzing programs written in C with **#ifdef** directives. The only basic data types are mathematical integers. The tool reports as output the upper and lower bounds of probabilities that the target assertion is satisfied or violated in all variants of the given family. The prototype tool is written in OCAML. All abstract operators and sound transfer functions for the polyhedral domain are provided by the APRON library [13]. The BDD domain which combines Boolean formulae and APRON domains is provided by BDDAPRON library [12]. The tool also calls the LATTE model counter [11] to determine the number of solutions to preconditions discovered by abstract lifted analyses.

All experiments are executed on a 64-bit Intel-CoreTM i5 CPU, Lubuntu VM, with 8 GB memory. The reported times represent the average runtime of five independent executions. We have implemented two versions of lifted analysis: one based on BDDs  $\mathbb{D}(\mathbb{F}, \mathbb{P})$ , and one based on tuples  $\mathbb{P}^{\mathbb{K}}$ . Thus, we evaluate the performances of our approach when using BDDs vs. tuples. In general, the chosen feature ordering makes a significant difference to the size of the obtained BDD. In this work, the ordering of features is syntactically directed, that is the features occurring earlier in the syntax of a program are smaller in the ordering. It is an interesting topic for future research to consider other heuristics for finding good orderings [17].

For our experiment, we use several C programs taken from the 8th International Competition on Software Verification (SV-COMP 2019) (https://svcomp.sosy-lab.org/2019) as well as from the abstract interpretation community [17, 18]. We have selected some numerical programs with integers that our tool can handle. We have manually added input sections and variability, and in some of the programs we have also defined target assertions. Then, we have analyzed those programs using our prototype static analyzer. Table 1 summarizes relevant characteristics for each benchmark: the source where it is taken from, the number of lines of code (LOC), and the number of features.

Table 1 shows the performance of our technique on a selected set of benchmarks. Regarding the preciseness of the results, we can see in the EXACT column that our tool gives exact results without any approximation very often ( $\sqrt{}$  means that the result is exact,  $\approx$  means the result is approximate). Note that the exact results are reported when the found lower and upper bounds for success and failure probabilities are the same. We obtain exact results in most of the cases due to the fact that we use the expressive and very precise polyhedral abstract domain. For BDD-based analysis, there are two columns. In the first column, TIME, we report the running time in seconds to analyze the given program family using BDDs. In the second column, IMPROVE, we report how many times a BDD-based analysis is faster than the corresponding analysis based on tuples. This way, IM-PROVE represents a measure showing how much sharing occurs in BDDs for each benchmark. We can see that all BDD-based analyses achieve significant speed-ups compared to the tuple-based analyses, which range from 5 to 15 times. We have also experimented with different domain sizes n of input variables (for n=10 and n=1000). Thus, n denotes the number of possible values per input variable. We observe that we obtain similar time performance results for n=10 and n=1000, mostly due to the fact that LATTE and APRON are largely insensitive to those values in terms of time.

#### **RELATED WORK**

A formal methodology for deriving tuplebased lifted analysis from existing single-program analysis phrased in the abstract interpretation framework has been introduced in [8]. Subsequently, a lifted analysis with improved representation via BDDs has been proposed [10]. This paper extends the previous works on lifted analysis [8, 10] by applying them in performing a specific type of probabilistic lifted analysis, that is the calculation of assertion probabilities. In particular, we combine the results obtained from lifted analyses and the model counting techniques to count the number of values for input variables that will lead to assertion satisfaction/violation. Hence, we put in practice the lifted analyses [8, 10] to solve a practical problem.

Probabilistic analysis of single programs has been used before [3–5]. The work [3] uses symbolic execution to calculate path probabilities by counting the number of solutions to a path condition. However, in presence of loops this approach loses precision, since it cannot enumerate all program paths but considers only a finite number of feasible paths. The work [4] performs a probabilistic analysis of open programs with undefined identifiers (e.g. calls to library functions) using symbolic game semantics and model counting. In the presence of loops and undefined functions, bounded exploration is also used to obtain a feasible analysis. In this work, we use abstract interpretation to analyze programs, thus we provide a complete treatment of loops. Moreover, while all above analysis [3–5] work on single program, here we consider program families.

#### CONCLUSION

In this work, we have presented a combination of forward and backward abstract lifted analyses for computing reliability of program families. In particular, we calculate the lower and upper bounds of probabilities that a given assertion is satisfied or violated for all variants of a program family. The BDDbased lifted domain provides a symbolic and very compact representation of lifted properties of program families, where the sharing of information is maximized. We evaluate the proposed lifted domains on several C product lines. We experimentally demonstrate the effectiveness of BDD-based lifted analyses vs. tuple-based lifted analysis.

We currently support only uniform distribution of input values within their finite discrete domains. In future, we plan to model imprecision in the input by different non-uniform distributions, such as Binomial, Poisson, etc [20]. Our focus here is on estimating probability for safety properties. An interesting direction for future work would also be to consider liveness properties (termination) and expectation queries [19]. Another way to speedup lifted analyses is via so-called variability abstractions [21, 22], which reduce the configuration space to something more tractable. Combining variability abstractions and BDD-representation would be interesting to consider in future.

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#### ЗА ПРЕСМЕТУВАЊЕ НА ВЕРОЈАТНОСТИТЕ НА ТВРДЕЊАТА КАЈ ФАМИЛИИ ОД ПРОГРАМИ

#### Александар С. Димовски

#### Факултет за информатички науки, Универзитет "Мајка Тереза", Скопје, Република Македонија

Висококонфигурабилни софтверски системи (фамилии од програми) се појавуваат во многу апликациски подрачја и од многу причини. Тие може да продуцираат потенцијално многу слични програми (варијанти) преку селектирање соодветни конфигурациски опции (особини) во компајлирачко време. Многу од овие конфигурабилни софтверски системи можат да примаат на влез и да манипулираат со несигурни податоци.

Во овој труд претставуваме еден метод за пресметка на веројатности на тврдења (assertions) во фамилии од програми со несигурни влезни податоци. Прво, користиме комбинација од нанапред и наназад фамилијарни анализи кои се базирани на апстрактна интерпретација за да се пронајдат неопходните предуслови за дадено тврдење да биде задоволено/незадоволено во сите варијанти од една фамилија на програми. Користиме фамилијарни анализи базирани на бинарни одлучувачки дијаграми (БДД-ја) и нумерички апстрактни домени (на пример, Полихедралниот домен) со чија помош наоѓаме нумерички инваријанти во секоја програмска локација. Второ, техниките за броење модели се искористени за да се најде бројот на решенија на пронајдените неопходни предуслови (кои се дадени во форма на линеарни ограничувања, т. е. линеарни неравенки). Овие броеви ги користиме за да ја процениме веројатноста дека целното тврдење е задоволено/незадоволено. Овој метод го имплементиравме во една прототип алатка и направивме нејзина евалуација на неколку интересни фамилии од Ц-програми.

**Клучни зборови:** статичка анализа преку апстрактна интерпретација; броење на модели; софтверски продуктни линии (фамилии од програми)

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Original scientific paper

#### TIMING OF INOCULATION WITH SELECTED WINE BACTERIA ON THE KINETICS OF MALOLACTIC FERMENTATION AND SENSORY PROPERTIES OF SYRAH WINES FROM THE REPUBLIC OF NORTH MACEDONIA

Goran Milanov<sup>1\*</sup>, Sibylle Krieger-Weber<sup>2</sup>, Anthony Silvano<sup>3</sup>, Ann Dumont<sup>4</sup>, Dushko Nedekovski<sup>1</sup>

<sup>1</sup>Ss. Cyril and Metodius University, Institute of Agriculture - Skopje, Republic of North Macedonia <sup>2</sup>Lallemand Korntal-Münchingen, Germany <sup>3</sup>Lallemand SAS, Blagnac, France <sup>1</sup>Lallemand, Montréal, Canada

e-mail: milnovg@yahoo.com

To improve the quality of the wine the use of selected strains of lactic acid bacteria become regular and important tool in modern wine making practice. As a result of metabolic activity of the lactic acid bacteria in the fermentation process the wines acidity is reduced and the wines flavour is more shaped. For the study four commercial LAB strains form the producer Lallemand were used in the fermentation of Syrah grapes: Lalvin VP41, O-MEGA, ML-Prime, PN4. The objective of this study was to determine the sensorial impact between co-inoculation and sequential application of four different lactic acid bacteria strains. From the obtained results co-inoculation samples resulted in higher level of esters and higher fruit intensity. Some strains contributed to more freshness and varietal characters of the wines and other increased the wine mouthfeel and red berry flavours.

Key words: Syrah grapes co-inoculation; lactic acid bacteria; kinetics; sensorial impact

#### **INTRODUCTION**

Malolactic fermentation (MLF) occurs in wine as a result of the metabolic activity of wine lactic acid bacteria (LAB). MLF reduces wine acidity and shapes wine flavour, both of which are considered to be beneficial to wine quality. Additionally, the use of selected strains of wine bacteria allows better control of the timeframe of L-malic acid degradation.

Since the quality of wine is the main objective of winemakers, the use of selected wine bacteria is more and more recognized as an important tool for winemakers leading the MLF process. Sensory studies show that flavour compounds produced by wine LAB bring recognizable changes to the flavour characteristics of wine [1–4]. Several studies show that different strains of wine LAB will have different sensory impacts in wines [1, 5–9]. The timing of the bacterial addition and the number

of cells in the wine after inoculation will also influence the sensory profile [10]

Although associated with some risk, MLF can be conducted by indigenous wine LAB present in the winery infrastructure, which may grow during alcoholic fermentation (AF) or immediately after its completion. Inoculation with selected wine LAB cultures allows for a better control over one of the last steps of vinification and traditionally inoculation was performed at the completion of AF. Beelman and Kunkee explored the possibility of inoculating wine LAB into juice along with the yeast used to conduct AF [11].

Current thinking identifies the following timing during wine production when selected wine LAB can be added (Figure 1).

• Co-inoculation: Selected wine LAB added 24 to 48 hours after yeast addition (or 48 to 72 hours if 80 to 100 ppm of  $SO_2$  is added at crushing)

• Early inoculation: Selected wine LAB added during active AF or at an approximate density of 1030/1040 kg/m<sup>3</sup> (8°/10°Brix)

• Post-alcoholic fermentation inoculation: At the end of, or just after, completion of AF

• Delayed inoculation: 2 to 6 months after completion of AF



Figure 1. Inoculation regimes for selected wine lactic acid bacteria (Adapted from Bartowsky, AWRI, 2010)

The tendency to harvest high maturity grapes, resulting in higher pH and alcohol wines, seems to be more favourable to the development of indigenous bacteria flora. To limit the development of unknown indigenous bacteria, co-inoculation is an interesting winemaking option. It is a good practice to suppress at an early stage the growth of undesirable wild bacteria that can produce negative metabolites which can affect the quality of the wines, either directly by the production of negative aroma active aromas (mousy off-flavour, volatile acidity), or precursors boosting the volatile phenol productions by *Brettanomyces*, or masking the fruity varietal characters of the wines due to the production of compounds such as biogenic amines and diacetyl or acetaldehyde.

Grapes contain various aroma precursor compounds, glycosides, particularly linalool, nerol, and geraniol, which play an important role in red wine aroma. Other compounds such as phenolic compounds (astringency, bitterness) and nor-isoprenoids are aroma enhancers and are also be influenced by the activity of glycosidases. Higher aldehydes can contribute to green, herbaceous and vegetative aromas. Recent studies of Ramón Mira de Orduña have shown that certain wine bacterial strains are able to degrade some of these aldehydes and may contribute to the reduction of green and vegetative aromas. Finally, diacetyl play a role in red wines as providing an element of complexity. Concentration of diacetyl is dependent on numerous parameters including wine bacteria strain used, the timing of inoculation and the citric acid content of the wines [12].

#### MATERIALS AND METHODS

## Production of Syrah wines from Macedonia with different wine bacteria

The climate in Macedonia is very suited for cultivation of red grape varieties. Due to good climatic conditions (a good ratio between the number of sunny days and rainfall), the grapes are with very good quality and are used exclusively for the production of premium wines for example from Syrah grape variety. Macedonian Syrah grape juice contains L-malic acid in the ranges of 0.5 to 2 g/l.

In order to obtain more balanced and microbiological stable wine with a refined aroma, this study was undertaken to investigate the influence of different wine L-lactic acid bacteria species and strains on the sensory quality of Macedonian Syrah wines. For the study, one yeast strain and four different strains of wine LAB were used and co-inoculation strategy was compared to inoculation post alcoholic fermentation.

#### Methodology

Mature and healthy Syrah grapes from the South East part of the Macedonia (Strumica vine-

growing district, Vardar River valley) were harvested by hand. The sugar content of the harvested grapes was 235 g/l; total acidity (tartaric acid) 5.3 g/l; L-malic acid 1.35 g/l and pH = 3.7.

The grapes were immediately destemmed and crush on a small electric crusher and 30 mg/l SO<sub>2</sub> was added. The grape must was divided into 5 stainless steel tanks of 30 kg each. After addition of 1 g/hl EX-V enzyme each modality was inoculated with selected active dry yeast Lalvin ICV D-254<sup>TM</sup> at 25g/hl. 24 hours after yeast addition four lots were inoculated with different wine bacteria strains as outlined below. The dosages that we used were 1g/hl for Lalvin VP41; O-MEGA and PN4 and 10g/hl for ML Prime as suggested by the manufacturer. The control sample was without bacteria inoculation.

• Control (Lalvin ICV D254<sup>TM</sup>)

•Variant 1 co-inoculation (Lalvin ICV D254<sup>TM</sup> + Lalvin VP 41<sup>TM</sup>)

• Vaiant 2 co-inoculation (Lalvin ICV D254<sup>™</sup> + O-MEGA<sup>™</sup>)

• Varant 3 co-inoculation (Lalvin ICV D254<sup>TM</sup> + ML Prime<sup>TM</sup>)

• Varint 4 co-inoculation (Lalvin ICV D254<sup>TM</sup> + PN4<sup>TM</sup>)

During the alcoholic fermentation (AF) the cap was plunged daily 3 times. Fermaid  $E^{TM}$  nutrient was added 15 g/hl at the temperature during fermentation did not exceed 25°C. L-malic acid was analysed every 3 days. The wine was pressed after 14 days of fermentation and left to settle for 2 days. After racking of the wine a complete chemical analysis was conducted. At the end of the alcoholic fermentation the control wine was divided in 5 equal parts and sequentially inoculated with the same bacteria strains previously used in the co-inoculation trial. Along with the different strains of LAB, a bacteria nutrition addition was also made with Opti'Malo<sup>TM</sup> 20 g/hl

• Control

• Variant 1 sequent. Lalvin VP  $41^{TM}$  + Opti'Malo<sup>TM</sup>

• Variant 2 sequent. O-MEGA<sup>TM</sup> + Opti'Malo<sup>TM</sup>

• Variant 3 sequent. ML  $Prime^{TM}$  + Opti'Malo<sup>TM</sup>

• Variant 4 sequent. PN4<sup>TM</sup> + Opti'Malo<sup>TM</sup>

#### Enzymatic L-malic acid analyses

L-malic and L-lactic acid concentrations were determined using Oenolab enzymatic kit on an Agilent 8453 UV-VIS spectrophotometer.

#### Analysis of wine volatile components

The analysis of the volatile components was carried out using Varian Inc GC-MS (Varian 3900 GC, Saturn 2100T MS and Autosempler CP 8400). The working parameter of the instrument and the liquid-liquid extraction was used for isolation of the volatile components from the wine samples. The analysis was performed according to the described method of Ivanova [13].

#### Quantitative descriptive analysis

The sensory descriptive analysis was performed according to the method of Ubigli. Seven wine experts were involved for the descriptive evaluation of the investigated wines. The panel proposed 11 descriptors for the final evaluation. All wine samples were evaluated during one tasting session. All results of the tasting were presented in Radar chart type [14].

#### Statistical Analysis

Wine aroma results obtained from the GC-MS analysis were statistically processed by statistical package SPSS 13.0.

#### **RESULTS AND DISCUSSION**

Fermentation performance and wine chemistry

The AF was completed after 8-10 days and the wine was racked after 14 days (for the extraction of phenolic components). Kinetics of alcoholic fermentation was regular and didn't differ between the modalities. Analytical data of the wines after alcoholic and malolactic fermentation are shown in Table 1.

TA are total acidity (expressed as tartaric acid), VA are volatile acidity (expressed as acetic acid).

Samples marked with "CO" were produced with co-inoculations; samples marked with "Seq" were produced with the post-alcoholic fermentation inoculations.

The total acidity (TA) of the Control sample was higher than the other treatments because it was made only with a partial MLF process. This sample contained 1.35 g/L residual malic acid. All other treatments had undergone complete malic acid degradation.

	Sp. Grav- ity 20/20	Alchool vol%	Total ex- tract g/l	TA g/l	VA g/l	ph	Free SO <sub>2</sub> mg/l	Total SO <sub>2</sub> mg/l
VP 41 <sup>TM</sup> - CO	0.9934	13.30	27.1	4.5	0.38	3.55	16.64	37.64
ML Prime <sup>TM</sup> - CO	0.9930	13.48	27.1	4.5	0.43	3.65	21.76	45.25
$Omega^{TM}$ - $CO$	0.9929	13,65	27.4	4.5	0.52	3.53	21.76	48.96
$PN4^{TM} - CO$	0.9934	13.48	27.9	4.4	0.51	3.62	28.00	55.12
$VP \ 41^{TM}$ - $Seq$	0.9930	13.74	27.9	4.4	0.43	3.64	32.00	55.12
ML Prime <sup>TM</sup> - Seq	0.9932	13.56	27.9	4.5	0.48	3.55	25.60	44.00
Omega <sup>TM</sup> - Seq	0.9929	13,65	27.4	4.7	0.45	3.50	25.60	52.32
PN4 <sup>TM</sup> - Seq	0.9928	13.74	27.4	4.7	0.52	3.55	21.76	48.52
Control	0.9930	13.65	27.4	5.2	0.58	3.64	25.60	51.25

Table 1. Physicochemical analysis of the wines after alcoholic and malolactic fermentation

The results in Figures 2 & 3 shown that in all the treatments with co-inoculation, the L-malic acid was metabolized into L-lactic acid except in the control wine where L-malic acid was unchanged. The MLF kinetics shown that *L. plantarum* ML Prime<sup>TM</sup> was very effective and able to degrade the L-malic acid within 6 days, followed by *O. oeni* PN4<sup>TM</sup> strain, which started L-malic acid degradation after a short lag phase, and completed MLF within 10 days. The other two LAB strains were slightly slower but still very efficient for the L-malic acid degradation. They finished the MLF within 17 days.

Using the traditional inoculation technique (sequential), inoculation (sequential) with selected wine LAB after alcoholic fermentation, kinetics of malic acid degradation had been almost identical between the for selected wine LAB strains. Although not recommended for sequential inoculation in red wines, the *L. plantarum* strain started the malic acid degradation faster than the *O. oen* i strains, but all LAB strains degraded malic acid within 3 weeks (Figures 2).



Figure 2. Kinetics of degradation of L-malic acid by four different selected wine lactic acid bacteria strains by co-inoculation and postalcoholic fermentation (sequential) inoculation



Figure 3. Kinetics of L-lactic acid formation by four different selected wine lactic acid bacteria strains by co-inoculation and post-alcoholic fermentation (sequential) inoculation

#### Wine aroma and sensory analyses

Volatile aroma compounds were analysed by gas chromatography-mass spectrometry (GC-MS). The results are presented in Table 2. From the obtained result we can see that statistically proven differences were found between the variants for different wine aromas. For the content of 2-phenylethanol the lowest level was analysed in the Co-inoculated variant with VP-41 (37921µg/l) and the highest level was analysed in Co and Seq-inoculated variants with PN4 strain (49652 and 49184 µg/l, respectively). For isoamyl acetate and 2-phenylethyl acetate the Co-inoculated samples had statistically proven higher values than the Sequentional and Control variants with the exception of the Co-inoculation variant with VP-41. For ethyl hexanoate two groups were formed. First group was with highest statistically proven values. It included the variants with Co-inoculation VP-41 and PN4 (366,9 and 357,1 µg/l, respectively). The second group was with lowest value. It included the Sequentional inoculation with ML Prime (292,2  $\mu$ g/l).

Bacteria co-inoculation overall resulted in a higher increase of ethyl esters with the exception of phenyl ethanol in the wine co-inoculated with Lalvin VP  $41^{TM}$  and ML Prime<sup>TM</sup>.

For the C13 nor-isoprenoids statistically proven differences were analysed for  $\alpha$ -ionone for the variant Seq. inoculation with ML Prime (0.03 µg/l), for  $\beta$ -damascenon the highest level was analysed for Co-inoculation with VP-41. There were some changes in the terpene alcohols following MLF (increase in geraniol and linalool, decrease in citronellol) however, little impact was observed between the strains or timing of inoculation.

Overall the co-inoculated wines had higher levels of fruity esters compared to the wines with sequential MLF and the control wine. 2-phenyl ethanol, a major volatile compound formed during the AF decreased in concentration only for co–inoculated wines with Lalvin VP 41<sup>TM</sup> and ML Prime<sup>TM</sup>. The concentrations of isoamyl acetate and 2-phenyl acetate increased with ML, overall higher with co-inoculation, especially with strains PN4<sup>TM</sup>, O-MEGA<sup>TM</sup> and ML Prime<sup>TM</sup>

The 2016 Syrah wines from Strumica vinegrowing district (Vardar River valley) were accessed by a sensory panel (Figures 4 and 5) which highlights how these wines have been shaped during MLF with using of different selected wine bacteria strains. Figure 4 shows the wines, which have been co-inoculated (24 hours after the yeast inoculation). There is a clear sensory impact of the specific wine LAB strain. For example, the wine inoculated with LAB strain O-MEGA<sup>TM</sup>, was described as more acidic, with more body balance and red fruit aromas. This corresponded with the potential of O-MEGA<sup>TM</sup> to protect the varietal aromas, to increase the aromatic intensity and bring freshness to Syrah wine resulting from grapes with high maturity. This result was in contrast to the control wine, which was dominated by bitterness and astringency. Overall co-inoculated wines were fruitier which correlated with the overall higher fruity ester concentrations obtained in these wines. This was in agreement with other studies too [15, 16].

	Higher alcohol							Ester	s					
Analyzed aroma component	2-phenylethanol	isoamyl acetate	2-phenylethyl acetate	ethyl decanoate	ethyl hexanoate	ethvl octanosta	Cury I Octanoate	ethyl butanoate		ethyl 2-hydroxypropanoate	ethyl 3-hydroxybutanoate	ethyl 2-methylbutanoate	ethyl 2-methylpropanoate	ethyl 2-hydroxyisocaproate
Variants	(µg/l)	(µg/l)	(µg/l)	(µg/l)	(µg/l)	(µg	g/l)	(µg/l)		(µg/l)	(µg/l)	(µg/l)	(µg/l)	(µg/l)
Control	4383 c	671 d	31 c	29,6 bc	326,7 ab	154	,1 c	538,5 e	f 1	13684,3 i	585,3 a	13,6 a	106,4 ab	49,1 b
Co-inc. VP-41	37921 f	784 c	29,7 c	30,4 bc	366,9 a	174,	,9 b	654,8 c	: 7	70057,1 a	520,7 ab	10,6 a	87,2 b	56,8 ab
Co-inc. ML Prime	39832 e	1329 a	65,6 a	50,4 a	346,2 ab	194	,7 a	607,2 d	1 4	3078,9 g	381,2 b	13,1 a	94,1 ab	51,9 ab
Co-inc. Omega	41052 d	1194 b	55,6 b	32,9 bc	313,3 ab	172,	,8 b	717,4 t	<b>6</b>	51432,9 d	442,5 ab	13,6 a	105,8 ab	46,9 b
Co-inc. PN-4	49652 a	1118 b	49,9 b	36,1 bc	357,1 a	182,	6 ab	804,7 a	1 6	58033,4 b	520,9 ab	11,5 a	102,9 ab	46,8 b
sec. VP-41	43935 c	707 cd	33,4 c	26,9c	307,9 ab	136	,1 d	547,4 e	e 5	5182,6 e	583,3 a	12,5 a	100,6 ab	60,1 ab
Sec.ML Prime	45480 b	704 cd	32,7 c	33,7bc	292,2 b	154	,9 c	508,5 f	5	52497,6 f	585,5 a	13,1 a	102,3 ab	56,2 ab
Sec. Omega	43407 c	715 cd	32 c	38,1 b	317,7 ab	142,	8 cd	471,3 g	g 6	5190,6 c	549,9 b	12,6 a	100,6 ab	65,3 a
Sec. PN-4	49184 a	723 cd	32,1 c	32,2 bc	313,2 ab	142,	7 cd	553,6 e	e 3	31222,1 h	531,ab	13,1 a	110,9 a	54,3 ab
	(	C13-noriso	prenoids			Terpene alcohols								
Analyzed aroma component	1,1,6-trimethyl-1,2-dihydronaphtalene	α-ionone	β-damascenone	β-ionone	linallol	nerol	geraniol		citronellol	alpha terpineol	rose oxyde			
Variants	(µg/l)	$(\mu g/l)$	$(\mu g/l)$	(µg/l)	(µg/l)	(µg/l)	(µg/]	l) (µ	ıg/l)	(µg/l)	(µg/l)			
Control	0,048 b	0,017 b	5,1 b	0,22 a	6,8 cd	3,4 d	7,7 1	f 17	7,9 a	3,1 cd	0,12 a			
Co-inc. VP-41	0,041 c	0,021 b	5,3 a	0,14 a	19,1 a	4,4 ab	13,8	d 16	5,4 b	6,2 a	0,13 a			
Co-inc. ML Prime	0,03 f	0,029 a	3,4 d	0,11 a	5,7 d	3,7 cd	12,7	e 15	5,2 c	2,2 d	0,11 a			
Co-inc. Omega	0,027 g	0,025 b	3,9 c	0,11 a	6,1 cd	3,6 cd	12,4 g	ge 13	3,4 d	2,5 d	0,09 a			
Co-inc. PN-4	0,037 d	0,021 b	3,3 d	0,11 a	6,6 cd	4,3 ab	14,7	c 15	,7 bc	2,6 d	0,13 a			
sec. VP-41	0,046 b	0,028 b	4,8 b	0,24 a	8,7 b	3,5 d	14,5 0	cd 15	,5 bc	3,2 bc	0,08 a			
Sec.ML Prime	0,034 e	0,03 ab	4,9 b	0,23 a	8,1 bc	4,7 a	16,9	b 18	3,1 a	3,6 b	0,09 a			
Sec. Omega	0,042 c	0,027 b	4,9 b	0,20 a	8,9 bc	4,0 bc	19,8	a 16	5,4 b	3,6 b	0,09 a			
Sec. PN-4	0,054 a	0,018 b	5,1 b	0,19 a	8,9 b	4,3 ab	13,9 0	cd 18	3,6 a	3,6 b	0,11 a			

**Table 2.** Volatile aroma compounds ( $\mu g/L$ ) in x Syrah wines, vintage 2016 from Macedonia after malolactic fermentation by different selected wine LAB strain and two timing of inoculation



**Figure 4**. Sensory description of 2016 Syrah wine co-inoculated with 4 selected wine lactic acid bacteria strains compared to a control wine without MLF

Wine LAB strain PN4<sup>TM</sup> is recommended to bring more structure, creaminess and more red berry fruit sensations to wine, which was observed in this study with the sequentially inoculated Syrah wine (Figure 5). Again the control wine showed more astringency and bitterness than the wine sequentially inoculated wine LAB. The LAB strains had positive sensory impact on the body, structure and harmony of the wine and decrease the impact of herbal notes that can have a negative influence on the overall aroma of wines.



Figure 5. Sensory description of 2016 Syrah wine inoculated after alcoholic fermentation with 4 selected wine lactic acid bacteria strains compared to a control wine without MLF)

#### CONCLUSION

Today we have a range of reliable selected wine LAB strains available to the wine industry which do not only degrade malic acid to lactic acid in an acceptable time frame, but consistently produce favourable products with no defects. The choice of LAB strains provide an essential winemaking decision tool to fine-tune the sensory style of red wines through varied metabolism which is dependent on wine bacteria strain selected for the MLF through their esterase and glycosidase enzymes activities, as well as the citric acid metabolism. The study shown that the use of selected wine LAB strain can help to assure faster malolactic fermentation, regardless of MLF inoculation strategy, co- or sequentially inoculation.

In this study we showed that the ester profile of the wines was modified during the course of MLF in wine. The highest volatile ester concentrations were observed in the wines where bacteria had been inoculated 24 h after the yeast (co-inoculation). The success and convenience of selected MLB strains is due to their ability to produce desirable metabolites with minimal or no production of undesirable compounds.

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Co-inoculation resulted in higher ester levels and higher fruit intensity. Some strains contributed to more freshness and varietal characters, other strains increased mouthfeel and red berry flavours and all wines with malolactic fermentation were described as having lower acidity and astringency.

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#### ВРЕМЕ НА ИНОКУЛАЦИЈА СО СЕЛЕКЦИОНИРАНА ВИНСКА БАКТЕРИЈА ВРЗ КИНЕТИКАТА НА МАЛОЛАКТИЧКАТА ФЕРМЕНТАЦИЈА И СЕНЗОРНИТЕ КАРАКТЕРИСТИКИ НА ВИНА ОД СИРА ОД РЕПУБЛИКА СЕВЕРНА МАКЕДОНИЈА

#### Горан Миланов, Sibylle Krieger-Weber, Anthony Silvano, Ann Dumont, Душко Неделковски

<sup>1</sup>Земјоделски институт, Универзитет "Св. Кирил и Методиј", Скопје, Република Северна Македонија <sup>2</sup>Lallemand Korntal-Münchingen, Germany <sup>3</sup>Lallemand SAS, Blagnac, France <sup>1</sup>Lallemand, Montréal, Canada

За да се подобри квалитетот на виното, употребата на селекционирани видови млечно-кисели бактерии станува редовна и важна алатка во современата винарска практика. Како резултат на метаболичката активност на млечно-киселите бактерии во процесот на ферментација, киселоста на вината се намалува, а вкусот на вината е позаокружен. За студијата, во процесот на ферментација на грозјето од сортата *сира* беа користени четири комерцијални соеви ЈМБ од производителот Lallemand: Lalvin VP41, O-MEGA, ML-Prime, PN4. Целта на оваа студија беше да се утврди сензорното влијание помеѓу варијантите со коинокулација и секвенцијална апликација на четири различни соеви на млечно-кисели бактерии. Од добиените резултати, примероците со коинокулација резултираа со зголемено ниво на естри и поголем интензитет на овошни ароми. Некои од соевите придонесоа за поголема свежина и сортен карактер на вината, а други за зголемено времетраење на ефект на вкусот и аромат на црвени зрнести плодови.

Клучни зборови: коинокулација на грозје од сира; млечно-кисели бактерии; кинетика; сензорно влијание

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Original scientific paper

#### CONTENT OF EXCHANGEABLE CATIONS OF SOILS FORMED ON GYPSUM ROCKS IN THE REPUBLIC OF MACEDONIA

#### Marjan Andreevski<sup>1\*</sup>, Gjorgji Filipovski<sup>2</sup>

<sup>1</sup>Institute of Agriculture, Ss. Cyril and Methodius University, Skopje, Republic of Macedonia <sup>2</sup>Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia

#### \*e-mail: m.andreevski@zeminst.edu.mk

The current paper examines the content of exchangeable cations of soils formed on gypsum rocks in the Republic of Macedonia. The cation exchange capacity in gypsic rendzic leptosol ranges between 6.68 and 19.28  $\text{cmol}(+)\text{kg}^{-1}$  of soil while in gypsic pararendzina it ranges between 3.92 and 18.83 $\text{cmol}(+)\text{kg}^{-1}$  of soil. The cation exchange capacity decreases with profile depth in gypsic pararendzina, which is a result of the reduction of humus content. In both soil types, the exchangeable Ca is dominant in the adsorption complex, followed by Mg, whereas the occurrence of K and Na is minimal.

**Key words**: cation-exchange capacity; exchangeable cation; gypsum rocks; soil; gypsic pararendzina; gypsic rendzic leptosol

#### **INTRODUCTION**

Soils formed upon gypsum rocks are some of the least studied types of soil in our country. On a global scale they are poorly examined, too, with scarce data available. This is due to the narrow distribution of gypsum rocks on earth surface, which is a prerequisite for formation of these types of soil. According to [1], most of the landscapes where solid gypsum rocks occur are located in the northern hemisphere, primarily in Europe, less in Northern America and Asia. Owing to the distinctions in their morphological and chemical properties, soils constituted on gypsum rocks are divided into two groups, as follows: 1) soils of humid areas and 2) soils of semiarid continental and Mediterranean areas. The soils from the first group have been described in Russia, Poland, Germany and France while the semiarid variations have been described from Russia, Spain, Italy, the USA, Iran and Iraq. The soils to be dealt with in the current paper belong to the latter variation.

We [2] are the first to have conducted research into soils formed on gypsum rocks in the Balkan Peninsula. These soils are distributed in the vicinity of the villages of Dolno and Gorno Kosovrasti, Debar area, the Republic of Macedonia. A segment of the research referring to soil-forming conditions, morphological properties, genesis, evolution, classification, mechanical composition and a number of chemical properties was published in our preceding paper [3]. The current work will elaborate on the results from the study of content of exchangeable ions of gypsic rendzic leptosol and gypsic pararendzina for profiles identical with those observed in the earlier paper.

As mentioned above, there is very limited literature data concerning these types of soil, in particular data on the content of exchangeable ions. Therefore, we have set a goal to study the content of exchangeable ions of soils formed on gypsum rocks in the Republic of Macedonia. The content of exchangeable ions is an indicator of the conditions where soil genesis occurs, and it has a different impact both on the soil-genesis direction and on soil fertility, genesis, evolution and properties of soils formed on gypsum rocks.

Field research and laboratory analyses have been conducted in compliance with the established methods [4, 5].

Data on the content of exchangeable ions of soils formed on gypsum rocks have been published in foreign literature by [1, 6-8].

#### **RESEARCH RESULTS**

In the vicinity of the villages of Dolno and Gorno Kosovrasti (Debar area), 7 soil profiles on gypsum rocks (Map 1) were excavated, studied and morphologically described, whereof four profiles are gypsic rendzic leptosol with A-R profile and three profiles are gypsic pararendzina with A-AC-C profile.



Map 1. Profile location

#### Cation-exchange capacity

The cation-exchange capacity is dependent on the total clay quantity, character of clay minerals, humus content and on the reaction of the solution for extraction of exchangeable ions during their identification.

Table 1 and 2 comprise data on the cationexchange capacity of soils formed on gypsum rocks. The cation-exchange capacity of gypsic rendzic leptosol is 14.11 cmol(+)kg<sup>-1</sup> of soil on average varying from 6.68  $\mu$  0 19.28 cmol(+)kg<sup>-1</sup> of soil.

These large differences are due to the distinctions in the content of clay and humus. According to the classification provided by Penkov [9], the studied gypsic rendzic leptosol possesses medium cation exchange capacity, apart from prof. 8, which has a small cation exchange capacity.

 Table 1. Content of exchangeable cations of soils formed on gypsum rocks in the Republic of Macedonia (average values)

Horizon	Exchan	geable ca	tions in	cmol(+	Exchangeable cations in % of T							
	Ca <sup>2+</sup>	$Mg^{2+}$	$\mathbf{K}^+$	$Na^+$	S	Т	V%	$Ca^{2+}$	$Mg^{2+}$	$\mathbf{K}^+$	$Na^+$	
Gypsic rendzic leptosol												
А	11,32 2,27 0,30 0,22 14,11 14,11 80,00 16,02 2,35 1,											
					Gypsic p	ararendzi	na					
А	12,36	2,75	0,42	0,29	15,81	15,81	100,00	77,88	17,32	2,84	1,94	
AC	7,42	1,64	0,21	0,13	9,39	9,39	100,00	78,88	17,18	2,52	1,42	
С	3,26	0,69	0,07	0,03	4,05	4,05	100,00	80,40	17,03	1,83	0,74	

No	Horizon	Exchan	geable c	ations i	n cmol	(+)kg <sup>-1</sup> of	f soil		Exchang	eable cati	ons in %	of T
of prof	and depth in cm	Ca <sup>2+</sup>	$Mg^{2+}$	$\mathbf{K}^+$	$Na^+$	S	Т	V%	Ca <sup>2+</sup>	$Mg^{2+}$	$\mathbf{K}^+$	$Na^+$
-				(	Gypsic 1	endzic le	eptosol					
1	A 0-18	15.61	3.15	0.30	0.22	19.28	19.28	100	80.96	16.34	1.56	1.14
3	A 0-16	14.92	2.74	0.30	0.28	18.24	18.24	100	81.80	15.02	1.64	1.54
5	A 0-21	9.36	2.21	0.45	0.23	12.25	12.25	100	76.40	18.05	3.67	1.87
8	A 0-17	5.40	0.98	0.17	0.13	6.68	6.68	100	80.83	14.67	2.54	1.95
					Gypsic	pararen	dzina					
2	A 0-19	14.82	3.57	0.28	0.16	18.83	18.83	100	78.70	18.96	1.49	0.85
2	AC 19-32	9.83	2.33	0.09	0.11	12.36	12.36	100	79.53	18.85	0.73	0.89
6	A 0-15	13.08	2.52	0.52	0.36	16.48	16.48	100	79.36	15.29	3.15	2.18
6	AC 15-24	6.38	1.26	0.26	0.22	8.12	8.12	100	78.57	15.51	3.20	2.71
6	C 24-50	3.16	0.63	0.11	0.02	3.92	3.92	100	80.61	16.07	2.81	0.51
6	C 50-80	3.41	0.72	0.05	0.03	4.21	4.21	100	81.00	17.10	1.19	0.71
7	A 0-15	9.17	2.15	0.47	0.34	12.13	12.13	100	75.59	17.72	3.87	2.80
7	AC 15-28	6.04	1.32	0.28	0.05	7.69	7.69	100	78.54	17.17	3.64	0.65
7	C 28-43	3.20	0.72	0.06	0.04	4.02	4.02	100	79.60	17.91	1.49	1.00

Table 2. Content of exchangeable cations of soils formed on gypsum rocks in the Republic of Macedonia

The data on cation-exchange capacity in rendzina on hard limestones and dolomites from Jablanica Mt quoted by [10] are much higher compared to gypsic rendzic leptosol, and they come as a result of the higher content of clay and humus.

The cation-exchange capacity of gypsic pararendzina is the highest in the humusaccumulative horizon, and it is  $15.81 \text{ cmol}(+)\text{kg}^{-1}$  of soil on average for the type, varying from 12.13 to 18.83  $\text{cmol}(+)\text{kg}^{-1}$  of soil. The values of the cation exchange capacity decrease from the humusaccumulative towards the transitional horizon and the parent material. On average, the cation-exchange capacity in the transitional horizon amounts to 9.39 cmol(+)kg<sup>-1</sup> of soil, varying from 7.69 to 12.36  $cmol(+)kg^{-1}$  of soil, and in the parent material its average value is 4.05 cmol(+)kg<sup>-1</sup> of soil, varying from 3.92 to  $4.21 \text{ cmol}(+)\text{kg}^{-1}$  of soil. The cationexchange capacity becomes reduced with profile depth as a result of humus content decrease. On the basis of the aforementioned classification, humusaccumulative horizons of gypsic pararendzina and the transitional horizon of prof. 2 have medium cation exchange capacity; the transitional horizons of prof. 6 and 7 have a small cation exchange capacity while horizon C of prof. 6 and 7 has very little cation exchange capacity. Similar values for soils resembling our gypsic pararendzina have been reported by [6,8]. As maintained by [6], the cation exchange capacity in hor. A is 17, in hor. AC it is 16 and in hor. C it is  $5.1 \text{ cmol}(+)\text{kg}^{-1}$  of soil. Kliment'ev *et al.*[8] state values that tend to decrease with profile depth, and they are 15. 3, 11. 4 and 10.00 cmol(+)\text{kg}^{-1} of soil.

#### Content of Exchangeable Cations

Data on exchangeable base cations in soils formed on gypsum rocks are provided in tables 1 and 2.

Judging by the data from tables 1 and 2, it may be ascertained that in gypsic rendzic leptosol,  $Ca^{2+}$  is the overriding exchangeable base cation, followed by Mg<sup>2+</sup>, K<sup>+</sup> whereas Na<sup>+</sup> is the least present. The average content of exchangeable Ca<sup>2+</sup> is 11.32 cmol(+)kg<sup>-1</sup> of soil (5.4 to 15.61 cmol(+)kg<sup>-1</sup> of soil). Expressed in percentage of the cation exchange capacity, the exchangeable Ca<sup>2+</sup> is 80.00 % (76.4 to 81.8 %) on average.

 $Mg^{2+}$  is the second most represented exchangeable cation in the adsorption complex. The content of the exchangeable  $Mg^{2+}$  ranges between 0.98 to 3.15 cmol(+)kg<sup>-1</sup> of soil, the average is 2.27 cmol(+)kg<sup>-1</sup> of soil, or expressed in percentage of the cation exchange capacity - from 14.67 to 18.05 %, on average 16.02 %.

The exchangeable ions of K<sup>+</sup> and Na<sup>+</sup> are found in small quantities. The average content of exchangeable potassium amounts to 0.30 cmol (+) kg<sup>-1</sup> of soil, varying from 0.17 to 0.45 cmol (+) kg<sup>-1</sup> of soil, or expressed in percentage of the cation exchange capacity - on average 2.35 %, varying from 1.56 to 3.67 %. The content of exchangeable Na<sup>+</sup> is the lowest, and it is 0.22 cmol (+) kg<sup>-1</sup> of soil on average, with a variation interval from 0.13 to 0.28 cmol (+) kg<sup>-1</sup> of soil. Expressed in percentage of the cation-exchange capacity, the exchangeable Na<sup>+</sup> ranges from 1.14 to 1.95 %, on average 1.63 %.

If the content of exchangeable cations in gypsic rendzic leptosol and in rendzina on hard limestones and dolomites in Jablanica Mt is compared, the following will be established: both in gypsic rendzic leptosol and in rendzina on hard limestones and dolomites, the most represented base cation is calcium, then magnesium, potassium while sodium comes last. In gypsic rendzic leptosol because of the occurrence of CaCO<sub>3</sub> and gypsum in certain profiles, there is absence of exchangeable ions of H +Al while in rendzina on hard limestones and dolomites they are present. Therefore, base saturation percentage in gypsic rendzic leptosol is 100 % while in rendzina on hard limestones and dolomites it is 73.6 % on average.

Calcium is also the most prevailing in the adsorption complex of gypsic pararendzina. The average content in hor.A is the highest, and it is 12.36 cmol (+) kg<sup>-1</sup> of soil (9.17 to 14.82 cmol (+) kg<sup>-1</sup> of soil), the transitional horizon 7.42 cmol (+) kg<sup>-1</sup> of soil (6.04 to 9.83 cmol (+) kg<sup>-1</sup> of soil) and in hor. C 3.26 cmol (+) kg<sup>-1</sup> of soil (3.16 to 3.41 cmol (+) kg<sup>-1</sup> of soil). Expressed in percentage of the cationexchange capacity, the exchangeable calcium in hor.A is 77.88 % (75.59 to 79.36 %) on average, hor.AC 78.88 % (78.54 to 79.53 %) and hor.C 80.40 % (79.6 to 81 %). The amount of CaCO<sub>3</sub> and gypsum increases with depth of profile in gypsic pararendzina, coupled by a rise in the percentage of exchangeable calcium in the adsorption complex.

The reasons for the greater occurrence of calcium in the adsorption complex of gypsic rendzic leptosol and gypsic pararendzina are the following: on the one hand, in some horizons, CaCO<sub>3</sub> and gypsum occur in the profile and they saturate the adsorption complex with Ca, while, on the other hand, they neutralize all of the acids produced in the humification and mineralization process. The exchangeable property of calcium is greater than that of magnesium, which is the reason why it is harder to wash. In contrast to magnesium, it penetrates less in the crystal lattices of secondary clay minerals; hence, more remains for exchange.

Calcium is a major nutrient element in plant nutrition and it plays a significant role in creation of stable fine granular structure. Calcium converts phosphates in an insoluble form, thereby protecting them from washing. Magnesium comes second in terms of occurrence in the adsorption complex of gypsic pararendzina, too. The content of exchangeable magnesium is the highest in hor. A and it is 2.75 cmol (+) kg<sup>-1</sup> of soil (2.15 to 3.57 cmol (+) kg<sup>-1</sup> of soil) on average, in AC horizon 1.64 cmol (+) kg<sup>-1</sup> of soil (1.26 to 2.33 cmol (+) kg<sup>-1</sup> of soil) and in hor.C 0.69 cmol (+) kg<sup>-1</sup> of soil (0.63 to 0.72 cmol (+) kg<sup>-1</sup> of soil). Expressed in percentage of the cation-exchange capacity, the exchangeable Mg<sup>2+</sup> in hor. A is 17.32 % (15.29 to 18.96 %) on average, in hor.AC 17.18 % (15.51 to 18.85 %), and in hor.C 17.03 % (16.07 to 17.91 %).

Magnesium is also an essential nutrient element in plant nutrition. As claimed by [11], magnesium deficit has been noted in acid sandy soils, which contain less than 0.2 cmol (+) kg<sup>-1</sup> of soil of exchangeable magnesium. Per the data obtained regarding exchangeable magnesium in gypsic rendzic leptosol and gypsic pararendzina, the conclusion is that there is no risk of a deficit of the quoted nutrient element.

The exchangeable K<sup>+</sup> and Na<sup>+</sup> are found in minor amounts. Exchangeable potassium is in the third place in terms of occurrence in the adsorption complex of gypsic pararendzina. The content of exchangeable K<sup>+</sup> in hor. A in gypsic pararendzina is  $0.42 \text{ cmol}(+) \text{ kg}^{-1}$  of soil (0.28 to 0.52 cmol (+) kg<sup>-1</sup> of soil) on average, in hor. AC 0.21 cmol (+) kg<sup>-1</sup> of soil (0.09 to 0.28 cmol (+) kg<sup>-1</sup> of soil), and in hor. C 0.07 cmol (+) kg<sup>-1</sup> of soil (0.05 to 0.11 cmol (+) kg<sup>-1</sup> of soil). Expressed in percentage of the cationexchange capacity, the exchangeable K<sup>+</sup> in hor. A is 2.84 % (1.49 to 3.87 %) on average, in hor.AC 2.52 % (0.73 to 3.64 %), and in hor. C 1.83 % (1.19 to 2.81 %).

The exchangeable Na<sup>+</sup> comes last in terms of occurrence. In hor. A, exchangeable Na<sup>+</sup> is found 0.29 cmol (+) kg<sup>-1</sup> of soil (0.16 to 0.36 cmol (+) kg<sup>-1</sup> of soil) on average, in hor. AC 0.13 cmol (+) kg<sup>-1</sup> of soil (0.05 to 0.22 cmol (+) kg<sup>-1</sup> of soil), and in hor. C 0.03 cmol (+) kg<sup>-1</sup> of soil (0.02 to 0.04 cmol (+) kg<sup>-1</sup> of soil). Expressed in percentage of the cation-exchange capacity, the exchangeable Na<sup>+</sup> occurs in hor. A 1.94 % (0.85 to 2.8 %) on average, in hor. AC 1.42 % (0.65 to 2.71 %), and in hor. C 0.74 % (0.51 to 1.00 %). According to [8], for a profile resembling gypsic pararendzina, the exchangeable Na ranges between 1.7 and 2.1 % of the cation-exchange capacity.

Similar to gypsic pararendzina, in calcareous pararendzina from Ovče Pole, it is calcium that is the most represented cation in the adsorption complex, followed by magnesium while potassium and sodium occur in minimum amounts [10]. Goryachkin *et al.*[7] provide data about exchangeable calcium, magnesium and hydrogen for soils formed on pure gypsic rocks from the boreal belt. Different from our soils on gypsic rocks, those do not contain CaCO<sub>3</sub> in the solum given that it is absent from the parent material. Ca is the most common cation in these soils, followed by H while magnesium comes last. Lafuente *et al.*[6] report on data from Spain for a profile akin to our gypsic pararendzina. Like our gypsic pararendzina, carbonates are also found in this profile whereas Ca is the most common cation, followed by Mg, Na and K.

The values of exchangeable sodium in gypsic rendzic leptosol and gypsic pararendzina are not detrimental to plants and they do not cause peptisation of colloids.

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#### СОСТАВ НА РАЗМЕНЛИВИТЕ КАТЈОНИ НА ПОЧВИТЕ ОБРАЗУВАНИ ВРЗ ГИПСЕНИ СТЕНИ ВО РЕПУБЛИКА МАКЕДОНИЈА

#### Марјан Андреевски<sup>1</sup>, Ѓорѓи Филиповски<sup>2</sup>

<sup>1</sup>Земјоделски институт, Универзитет "Св.Кирил и Методиј", Скопје, Република Македонија <sup>2</sup>Македонска академија на науките и уметностите, Скопје, Република Македонија

Во овој труд е проучен составот на разменливите катјони на почвите образувани врз гипсени стени во Република Македонија. Капацитетот на атсорпција на катјони во гипсените црници се движи од 6,68 до 19,28  $\rm cmol(+)kg^{-1}$  почва, а во гипсените рендзини од 3,92 до 18,8  $\rm cmol(+)kg^{-1}$  почва. Во гипсените рендзини по длабочина на профилот се намалува капацитетот на атсорпција на катјони и се должи на намалување на содржината на хумус. И во двата почвени типа, во атсорптивниот комплекс разменливиот Са е доминантен, следи Mg, а K и Na се минимално застапени.

Клучни зборови: капацитет на атсорпција на катјони, разменливи катјони, гипсени стени, почва, гипсена рендзина, гипсена црница

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Original scientific paper

## URBAN AIR POLLUTION IN SKOPJE AGLOMERATION – TRAFIC VS BACKGROUND CASE

#### Dejan Mirakovski<sup>\*</sup>, Blazo Boev, Ivan Boev, Marija Hadzi Nikolova, Arijanit Reka, Tena Shijakova

University Goce Delcev, Štip, Republic of North Macedonia

\*e-mail: dejan.mirakovski@ugd.edu.mk

Extreme winter time air pollution episodes, fortify public concerns and put focus on air pollution as most important environmental problem in urban areas throughout the country. However, focused research efforts to derive information about pollution sources and the amount they contribute to ambient air pollution levels, are still missing, thus leaving room for dubious discussions and political, instead of scientifically based abetment strategies.

Having in mind importance of proper information on air pollution sources and utilizing the data collected during several different measurement's campaigns performed for city of Skopje, as much extensive additional lab works and modeling efforts, indicative source apportionment analysis was performed for two sites (receptors) within Skopje urban area, one source specific (traffic) and one background site.

Key words: air pollution; sources apportionment; PMF; traffic; background

#### **INTRODUCTION**

While the air pollution has become recognized globally as one of most important environmental and health problems that urban population face nowadays, Balkan capitols become largely "popular" as a urban areas with the worst air quality in Europe, with Sarajevo leading on the unofficial AirVisual list, as the sixth most "polluted" city in Europe region, with PM 2.5 yearly average of 38.4  $\mu$ g/m<sup>3</sup>. Other capitols in the region closely follow, with Skopje ranked as tenth with PM 2.5 yearly average of 34  $\mu$ g/m<sup>3</sup>, Pristina ranked as twelfth with PM 2.5 yearly average of 34  $\mu$ g/m<sup>3</sup>, Sofia (21) and Belgrade (45) with respective PM 2.5 yearly averages of 28.2 and 23.9  $\mu$ g/m<sup>3</sup>.

Limited in scope and scattered scientific data, leave room for dubious discussions about air pollution sources identification and their respective contribution, making source apportionment public and political deliberation, instead of scientifically sound modeling exercise. Reliable and quantitative information on air pollution sources is essential for the drafting and implementation of air quality plans, especially having in mind that abatement at the source is core principle of any air pollution control strategy (Directive 2008/50/EC).

Source contribution or so-called Source Apportionment (SA) procedure include deriving information about pollution sources and the amount they contribute to ambient air pollution levels, using one of the three main approaches: emission inventories, source-oriented models, and receptor-oriented models. Receptor-oriented models imply apportion of the measured mass of an atmospheric pollutant at a given site (the receptor) to its emission sources by using multivariate analysis to solve a mass balance equation Belis *et al.*[1].

The main types of receptor-oriented models include but are not limited to positive matrix factorization - PMF, principal component analysis – PCA, multivariate models, regression models and chemical mass balance (CMB) models, Viana *et al.* [2]. These tools have the advantage of providing information derived from real-world measurements, including estimations of output uncertainty, and are extensively used for the quantification of source contributions at local and regional scales all over the world [1]. Due to well developed and freely distributed software support for PMF and CMB, application of those tools steadily growth in last years with improved source resolution and accuracy.

Compiling information's collected over a few distinctive measurement's campaigns, performed for city of Skopje, as much broad extra lab works and modeling efforts, receptor models were constructed for two sites within Skopje urban area. Samples were taken according to standard gravimetric method (EN 12341:2014) using a low volume sampler and 47 mm PTFE filters. Chemical composition was determined using Fluorescent X-ray Spectrometer (Shimadzu EDX-900HS) according to EPA/625/R-96/010a IO-3.3 method, supported with multielement ICP-MS analysis. Seasonal and diurnal variation of PM10, PM2.5, NO<sub>2</sub> and CO were obtained with real time monitoring during the sampling campaigns using the Air Pointers (MLU Recordum, Austria), as much a UGD AMBICON independent monitoring network. Source apportionment was performed using EPA PMF 5.0 positive matrix factorization software package.

#### MATERIALS AND METHODS

As reported elsewhere, Mirakovski et al. [6], sampling was performed at two sites in Skopje central urban area, out if industrial or specific single source impacts (excluding traffic for roadside site). Sites were selected having in mind large spatial and temporal variation of air pollution, local topography, and meteorology, as much as references for leveling of traffic related pollutants concertation to the background within 150 m from the road, Pasquier & Andre [7]. Traffic exposed site was located within 2 meters from Ilindenska boulevard at City of Skopje Administration Buildings backyard, while background location was located at eastern corner of Ministry of Agriculture and Forestry building, facing the border of Skopje central park (Figure 1). Roadside site, experience mostly triple traffic frequency at any given day of the monitoring campaigns.



Figure 1. Sampling locations in Skopje urban area

#### Sampling

Both sites were equipped with sequential dust sampling systems PNS 16T-3.1 (Comde Derenda, Germany) with 16/18 filter cassettes for continuous collection of particulate matter and Air Pointers (MLU Recordum, Austria) for real time monitoring of PM10, PM2.5, NO<sub>2</sub> and CO using compliance or equivalent methods.

Sampling was performed at 2.2 meters height, continuously during at least 14 consecutive days in

each season, starting from November 8–21.2018, January 18–31.2019, May 6–27.2019 and July 13–27.2019.

#### Gravimetry and elemental analysis

Particulate (PM10) samples were collected on 47 mm PTFE filters and handled and measured gravimetrically fully in line with recommendation given in EN 12341:2014 Ambient air - Standard gravimetric measurement method for the determination of the PM10 or PM2,5 mass concentration of suspended particulate matter. Quality control was performed fully in line with the requirements of EN 12341:2014 and measurement uncertainties were calculated following GUM concept (expanded relative uncertainty  $\leq 11.4$  %).

Elemental composition was measured by the energy dispersive X-ray fluorescence (EDXRF) using Fluorescent X-ray Spectrometer (Shimadzu EDX-900HS, Japan) for determination of Na, Cl, K, Ca, Mn, Fe, Ni, Cu, Zn, As, Cd, Pb, Si and S fully in line with EPA/625/R-96/010a, Method IO-3.3 Determination of Metals in Ambient Particulate Matter Using X-Ray Fluorescence (XRF) Spectroscopy. Measurement uncertainties were calculated based on blank and sampled filter concentrations. Expanded relative uncertainty varies for different elements between 5.2 % and 17 %.

Black Carbon or Elemental Carbon was analyzed with SootScan<sup>TM</sup> Model OT21 Optical Transmissometer Magee Scientific with dual wavelength light source (880nm providing the quantitative measurement of Elemental Carbon in PM, and a 370nm for qualitative assessment of certain aromatic organic compounds), by applying EPA empirical EC relation for TEFLON FRM filters. Measurement uncertainty was by convention set at 10%.

#### **PMF** Methods

Source Apportionment (SA) studies are usually done using one of three main methods: pollution inventories, source-oriented models and receptororiented models. As Belis et al. explain [1], receptor-oriented models apportion the measured mass of an atmospheric pollutant at a given site (receptor), to its emission sources by using multivariate analysis. Receptor models, supported by freely distributed software packages, have gained considerable popularity in recent years, with the particulate matter as chosen metric [2]. Source contribution/apportionment of PM10 mass by Positive Matrix factorization was performed using the EPA PMF version 5.0. program, in accordance with the user's guide [8].

Positive Matrix Factorization (PMF) is a receptor model, developed by Dr. Pentti Paatero (Department of Physics, University of Helsinki) in the middle of the 1990s [8], in order to develop a new method for the analysis of multivariate data that re-

solved some limitations of the PCA [9]. One of the main positive aspects is the use of know experimental uncertainties as input data which allow individual treatment of matrix elements and can accommodate missing or below-detection-limit data that are a common feature of environmental monitoring [10]. PMF results have a quantitative nature and therefore it is possible to obtain the composition of the sources determined by the model [12]. Concentration and uncertainty data matrices were compiled as recommended in PMF 5.0 Fundamentals and User Guide [8]. In total 20 base runs were performed, changing between 3 to 6 factors and base random seed with 0 % extra modelling uncertainty. Using the calculated sound to noise (S/N) ratios as recommended, all variables were categorized as "Strong".

#### Results and discussion

In order to gain overview of the data and explore the relationships between variables, basic statistic tests were performed, including, time trends, central and dispersion statistics, correlation matrices. As expected, temporal data variability was extremely high, with maximum values for most (if not all) contaminants included in the monitoring, displayed exclusively during the autumn/winter season. Even simple overview of time trends for suspended particulates PM10 concentration, confirms that daily averages above the limits are common for heating season only, while the same are well within the limits for spring and summer season (Figure 2). This is also the case for fine particulates fraction PM 2.5, nitrogen dioxide and elemental carbon concentrations.

Time trends also reveal distinct diurnal cycles during the high pollution episodes. Specific bimodal pattern, with two peaks, one in the morning and one in the late evening are frequently found. Such patterns could be driven with natural changes in boundary layer height but are also in direct conjunction with patterns of home heating usage, which also peaks in the morning and evening hours [6]. Similar diurnal patterns are reported elsewhere, for regions where domestic wood combustion for home heating is known to be a significant contributor to PM10 concentrations during the winter [14, 15].



Figure 2. 24 h average for PM10 – indicative values 2019

Correlation matrices exhibit especially high correlation value (> 0.9) between suspended particulates (PM10 and PM 2.5) concentrations at both locations, as much as between concentrations of different fractions at same locations (> 0.95). Similar, although a bit lower correlation values were found for other species including nitrogen dioxide, elemental carbon, and carbon monoxide (Table 1). However, seasonal data analysis reveal that high correlation values are specific only for autumn/winter season and not for spring/summer period. Very specific is the strong correlation between particulates and background carbon monoxide concentration, frequently used as a maker for low efficient combustion processes emissions [13], found also only during the autumn/winter season.

In order to fully investigate different sources contribution, data collected for coarse particulate

fraction and chemical composition were used to develop receptor model's at both sites, traffic exposed and the background site. As for each site, only 54 valid samples stretched over a 12-month period were available, PMF exercise should be seen as indication for dominant sources and cannot replace full scale source apportionment study. Low reconstructed mass percentages (around 30 %), mostly due to limited analytical exercise which does not included all usual components of ambient air particulates, like often dominant water-soluble ions (NH4<sup>+</sup>, SO4<sup>2-</sup> и NO<sub>3</sub>-), should also be taken in account for any further usage of data presented. Statistical description of the input data including average, maximum, and median concentrations of species used for source apportionment, as well as standard deviations, average uncertainties and limits of detection are given below (Table 2).

Full year data		Traf	Back	Traf	Back	Traf	Back	Traf	Back	Traf	Back
		PM 10 (µg/m <sup>3</sup> )		PM 2.5 (μg/m <sup>3</sup> )		NO2 (µg/m <sup>3</sup> )		CO (µg/m <sup>3</sup> )		EC (µg/m <sup>3</sup> )	
Traf	PM 10 (μg/m <sup>3</sup> )	1	0.91	0.97	0.91	0.76	0.86	0.51	0.80	0.89	0.81
Back	PM 10 (μg/m <sup>3</sup> )	0.91	1	0.93	0.98	0.78	0.86	0.59	0.84	0.99	0.92
Traf	PM 2.5 $(\mu g/m^3)$	0.98	0.93	1	0.94	0.80	0.88	0.55	0.83	0.92	0.84
Back	PM 2.5 (µg/m <sup>3</sup> )	0.91	0.98	0.94	1	0.77	0.85	0.62	0.85	0.93	0.93
Traf	NO2 $(\mu g/m^3)$	0.76	0.78	0.81	0.77	1	0.88	0.35	0.74	0.76	0.66
Back	$\frac{100}{MO2}$ (µg/m <sup>3</sup> )	0.86	0.86	0.88	0.85	0.88	1	0.48	0.83	0.83	0.75
Traf	CO (mg/m <sup>3</sup> )	-0.31	-0.22	0.09	0.08	0.54	-0.12	1	0.19	-0.69	-0.42
Back	CO (mg/m <sup>3</sup> )	0.80	0.84	0.83	0.85	0.74	0.83	0.72	1	0.87	0.82
Traf	EC $(\mu g/m^3)$	0.89	0.91	0.92	0.92	0.76	0.83	0.66	0.87	1	0.92
Back	EC (µg/m <sup>3</sup> )	0.81	0.91	0.84	0.93	0.66	0.75	0.68	0.82	0.92	1

Table 1. Correlation matrix – full year data 2018/19

 Table 2. PMF Input data

Valid data	Unit	Traffic	Back.	Traffic	Back.	Traffic	Back.	Traff/Back	Traff/Back
(N=54)		Min		Max		Avg		Uncertain.	Detection limit
Na (PM10)	$\mu g/m^3$	0.020	0.020	0.624	0.574	0.077	0.069	0.0020	0.0019
Cl (PM10)	$\mu g/m^3$	0.004	0.042	0.049	0.468	0.014	0.144	0.0014	0.0018
K (PM10)	$\mu g/m^3$	0.054	0.054	2.216	2.097	0.481	0.403	0.0010	0.0010
Ca (PM10)	$\mu g/m^3$	0.036	0.059	2.911	3.119	1.212	1.133	0.0021	0.0012
Mn (PM10)	$\mu g/m^3$	0.003	0.002	0.205	0.108	0.027	0.019	0.0044	0.0051
Fe (PM10)	$\mu g/m^3$	0.068	0.033	1.513	1.086	0.700	0.428	0.0071	0.0043
Ni (PM10)	$\mu g/m^3$	0.001	0.002	0.075	0.055	0.014	0.013	0.0016	0.0001
Cu (PM10)	$\mu g/m^3$	0.003	0.005	0.196	0.157	0.018	0.024	0.0041	0.0051
Zn (PM10)	$\mu g/m^3$	0.001	0.001	0.401	0.391	0.035	0.041	0.0061	0.0019
As (PM10)	$\mu g/m^3$	0.000	0.000	0.001	0.001	0.000	0.000	0.0003	0.0002
S (PM10)	$\mu g/m^3$	0.538	0.483	6.294	5.382	1.755	1.657	0.0124	0.0124
Pb (PM10)	$\mu g/m^3$	0.001	0.001	0.140	0.271	0.019	0.046	0.0004	0.0005
Si (PM10)	$\mu g/m^3$	0.059	0.059	0.658	0.918	0.178	0.201	0.0061	0.0012
PM10	$\mu g/m^3$	16.0	14.0	187.3	156.0	52.2	48.0	3	3.0
PM 2.5	$\mu g/m^3$	4.1	5.0	174.0	146.0	36.3	36.1	2	3.0
EC (PM10)	$\mu g/m^3$	3.8	3.0	43.6	43.6	15.1	14.5	0.0752	0.0100

Preforming multiple PMF runs to elemental data, optimal solution with 4 factors was obtained. Factors were identified as:

- different forms of biomass burring (open fires, small boilers and residential stoves) specific for high EC content, K, Cl and S,

- industrial sources with Ni, Si, Na, Cu and As,

 $\ \$  - traffic source specific for Zn, Cu, Mn and EC, as much as

- crustal sources which usually include Si, Ca and Na.

Some of the elements have contribution in several sources, as some processes, like resuspending road dust or combustion sources, contribute to a mixed source profiles (crustal matter Si, Ca and Na in traffic or EC in traffic, biomass burning and industrial emissions). Receptor models developed using EPA PMF 5.0. software, delineate specific sources contribution in coarse particulates fraction PM10, for both locations separately. As shown below (Figure 3) for traffic exposed location, largest contribution has by far come from different forms of biomass burning (69 %), followed by traffic with 22 %, industrial at 8 % and crustal dust with 1 %. Background location (Figure 3) experience similar impacts, having biomass burning as dominant contributor with almost 72 %, traffic with 14 %, industrial sources with 12 % and crustal dust with 2 %.



Figure 3. Factor contributions for PM10

#### CONCLUSIONS

Specific temporal variations (seasonal and diurnal) and correlations between different pollutant species at both locations clearly indicate domination of background sources compared to specific sources like traffic, while indicating high influence of low efficient combustion sources like residential wood stoves, open fires, and small boilers.

At both sites monitored, average yearly concentration was determined above the limits for coarse (PM10) and especially fine particulate (PM 2.5) fractions, only due to extremely high averages over the autumn/winter season, with same well within the limits out of heating season. While such pollution patterns could be explained with natural changes in boundary layer height during the cold whether season, direct conjunction with patterns of home heating, which also peaks in the morning and evening hours, is more than obvious.

In addition, source apportionment performed using Positive Matrix Factorization, clearly identify biomass burring as single dominant source at both location with high 69 % at traffic site and 72 % at background site, with no direct specific source impact. Such high contribution from biomass burning is not surprising, having in mind Skopje agglomeration emission inventory for reference 2014, where domestic heating participates with 91 %, in total PM10 emissions, while industry, energy production, traffic, waste management, agriculture and construction have altogether about 9 %, FMI & MOEPP [16]. Acknowledgement. Authors wish to acknowledge assistance from City of Skopje and Farmahem Environmental Lab for their support and participation in sampling and data collection process.

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#### ЗАГАДУВАЊЕ НА ВОЗДУХОТ ВО ГРАД СКОПЈЕ – СПОРЕДБА НА ПОЗАДИНСКА И НА ЛОКАЦИЈА ИЗЛОЖЕНА НА СООБРАЌАЈ

Дејан Мираковски, Блажо Боев, Иван Боев, Марија Хаџи Николова, Аријанит Река, Тена Шијакова

#### Универзитет "Гоце Делчев", Штип, Република Северна Македонија

Честите епизоди на екстремно загадување на воздухот во текот на зимските месеци, несомнено привлекуваат големо внимание и загриженост од јавноста, што веројатно го прави аерозагадувањето веројатно најважен еколошки проблем во урбаните средини ширум нашата држава. Но, за жал, речиси и да нема истражувачки напори, кои би биле фокусирани кон обезбедување на целосни информации околу поедините извори и нивното учество во вкупното загадување. Ваквите состојби, практично го лимитираат капацитетот на сите стратегии за решавање на проблемите со аерозагадувањето, кои наместо на научни се базираат на политички решенија.

Имајќи ја во предвид важноста на правилните информации за изворите на загадување на воздухот, а врз основа на податоците собрани во неколкукратни мерни кампањи во урбаната зона на град Скопје, како и

на дополнителни напори за хемиска карактеризација и конструкција на т.н. "рецепторни" модели, беа изработени индикативни студии за пропорционирање на поедините извори на две локации во Скопје, една изложена на интензивен сообраќај и една позадинска урбана локација.

Клучни зборови: загадување на воздухот; пропорционирање на поедини извори; позитивна факторизација; сообраќајна и позадинска локација

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Review

#### ADDITIVE SEMIGROUPS OF INTEGERS. EMBEDDING DIMENSION OF NUMERICAL SEMIGROUPS

#### Violeta Angjelkoska, Dončo Dimovski

Faculty of Informatics, FON University, Skopje, Republic of North Macedonia Macedonian Academy of Sciences and Arts, Skopje, Republic of North Macedonia

e-mail: violeta.angelkoska@fon.edu.mk, ddimovskd@gmail.com

We characterize the embedding dimension of numerical semigroups in the same manner as additive semigroups of integers are characterized in [1]. Moreover, we give a particular characterization of the Frobenius number of numerical semigroups with embedding dimension less than or equal to 3.

Key words: numerical semigroups; embedding dimension; Frobenius number

#### INTRODUCTION

This paper has been motivated by the results about the structure of additive semigroups of integers (Dimovski, [1]), geometric description of finitely generated subsemigroups of the additive semigroup  $\mathbb{N}^n$  (Dimovski and Hadži - Kosta Josifovska, [2]) and the description of finitely generated additive subgroups of  $\mathbb{Z}^n$  (Hadži - Kosta Josifovska and Dimovski, [3]).

The main results stated in these papers are the following:

**Theorem 1.1.** (Theorem 1.2. in [1]) Let *G* be a semigroup consisting of positive integers. Let *n* be the smallest integer in *G*, *d* the greatest common divisor of the elements of *G* and n = kd. Let us denote by  $A_i$ the set of all the elements in *G* whose remainder after division by *n* is *id*, i.e.

 $A_i = \{a | a \in G, a = nt + id, t \in \mathbb{N}\}.$  Then:

(*i*)  $G = A_0 \cup A_1 \cup ... \cup A_{k-1}$ , the union is disjoint. (*ii*) There exist  $1 = a_0, a_1, ..., a_{k-1}$ , such that

$$A_{i} = \{tn + id | t \ge a_{i}\} \text{ and} \\ a_{i} + a_{j} \ge \begin{cases} a_{i+j}, & i+j < k \\ a_{i+i-k} - 1, & i+j \ge k \end{cases}$$

(*iii*) If  $m_i = a_i n + id$ , then  $\{n = m_0, m_1, ..., m_{k-1}\}$  is a set of generators for *G*. (*iv*) Let

 $b = max\{a_0, a_1, \dots, a_{k-1}\},$   $s = max\{i|a_i = b\} \text{ and } c = (b-1)k + s + 1.$ Then

 $(c-1)d \notin G$  and  $\{td|t \ge c\} = G_* \subseteq G$ . (We say that  $G_*$  is the *regular part* of G.)

**Theorem 1.2.** (Theorem 2.1. in [1]) Let  $\alpha$  be a congruence on *G* and  $\alpha \neq \Delta_G$  ( $\Delta_G$  is the equality on *G*). Then there exist  $m, s_0, s_1, \dots, s_{k-1} \in \mathbb{N}$  such that: (*i*)  $a\alpha b \Rightarrow m | a - b$ .

(*ii*)  $(\forall t \in \mathbb{N}_0) [(s_i + t)n + id]^{\alpha}$  is an infinite class, and, for every  $v \in A_i$ ,  $v < s_i n + id \Rightarrow v^{\alpha}$  is a finite class for  $0 \le i \le k - 1$ .

(*iii*) The integers  $s_i$  satisfy the following conditions:

$$s_{i} \ge a_{i}, \\ s_{i} + a_{j} \ge \begin{cases} s_{i+j}, & i+j < k \\ s_{i+j-k} - 1, & i+j \ge k \end{cases}$$

**Theorem 1.3.** (Theorem 2.1. in [2]) An additive subsemigroup *G* of  $\mathbb{N}^n$  for n > 1 is finitely generated if and only if *G* is a subset of *Cone*(*A*) for some subset *A* of *G*.

Theorem 1.3. shows the major difference between the structure of additive subsemigroups of  $\mathbb{Z}^n$  for n > 1 and additive subsemigroups of  $\mathbb{Z}$ , since any additive subsemigroup of  $\mathbb{Z}$  is finitely generated. For better understanding of the additive subsemigroups of  $\mathbb{Z}^n$  a good description of the additive subgroups of  $\mathbb{Z}^n$  is given in [3].

Four years ago, we came across two papers about numerical semigroups (Semigroup Forum, see [4],[5]). We found out that they are in fact semigroups of nonnegative integers, whose greatest common divisor of their elements is 1.

Later, we found out that there are a lot of papers about numerical semigroups (see [6] - [13]), discussing the following notions: multiplicity, conductor, Frobenius number, embedding dimension, gaps, genus, etc. and also theorems analogous to Theorem 1.1, but not to Theorem 1.2.

With the notions as in Theorem 1.1, when d = 1,  $G \cup \{0\}$  is a numerical semigroup, whose multiplicity is n, conductor is c, the gaps are all the numbers tn + i, for  $t < a_i$ , the genus is  $\sum_{i=0}^{n-1} a_i$  and the Frobenius number is c - 1.

The notion of embedding dimension is not considered in [1]. The aim of this paper is to characterize the embedding dimension of numerical semigroups in the same manner as additive semigroups of integers are characterized in [1]. Moreover, using this characterization, we obtain an explicit form for the Frobenius number of numerical semigroups with embedding dimension less than or equal to 3.

Further on, instead of the term additive semigroups of nonnegative integers, we use the term numerical semigroups. Thus, a numerical semigroup *G* is a proper nonempty subset of  $\mathbb{N}_0$ , closed under addition, containing 0 and whose complement is finite, i.e.  $\mathbb{N}_0 \setminus G$  is finite. We say that a set

$$S = \{n_1, n_2, \dots, n_t\} \subseteq \mathbb{N}$$

is a set of generators for *G*, denoted by  $G = \langle S \rangle$ , if the elements of *G* are linear combinations of  $n_1, n_2, \ldots, n_t$  with nonnegative integer coefficients.

The condition (*iii*) in Theorem 1.1. implies that every numerical semigroup has a finite set of generators. Moreover, it has a unique minimal set of generators ([4]). The cardinality of the minimal set of generators for *G* is called *embedding dimension* of *G*, denoted by ed(G). The smallest number in the minimal set of generators is called *multiplicity* of *G*, denoted by *n*. The largest number not belonging to a numerical semigroup *G* is called *Frobenius number* of *G*, denoted by F(G). The set  $\mathbb{N}_0 \setminus G$  is known as the set of gaps of *G*. Its cardinality is called *genus* of *G*, denoted by g(G).

In this paper a numerical semigroup *G* will be denoted by G = [n, A], where *n* is the multiplicity of *G* and

$$A = \{1 = a_0, a_1, \dots, a_{n-1}\},\$$

where  $a_0, a_1, \ldots, a_{n-1}$  are as in Theorem 1.1.

#### SOME PRELIMINARY NOTIONS AND RESULTS

The addition of integers modulo *n* will be denoted by  $\oplus$  and the additive group of integers modulo *n* will be denoted by  $(\mathbb{Z}_n, \oplus)$ . If  $X \subseteq \mathbb{Z}_n$ , the subgroup of  $(\mathbb{Z}_n, \oplus)$  generated by *X* will be denoted by < X >. The subtraction of integers modulo *n* will be denoted by  $\ominus$ . The multiplication of integers modulo *n* will be denoted by  $\odot$ . For  $i_1, \ldots, i_k \in \mathbb{Z}_n$  and  $k \in \mathbb{N}$ , the integer part  $\left[\frac{i_1 + \ldots + i_k}{n}\right]$  will be denoted by  $[n; i_1, \ldots, i_k]$ , i.e.

$$[n; i_1, \dots, i_k] = \left[\frac{\iota_1 + \dots + \iota_k}{n}\right].$$

**Lemma 2.4.** Let  $n, k, t \in \mathbb{N}$ ,  $i_u, j_v \in \mathbb{Z}_n$  for  $1 \le u \le k, 1 \le v \le t$ ,  $j = i_1 \oplus \ldots \oplus i_k$  and  $s = j_1 \oplus \ldots \oplus j_t$ . Then:

 $(i) [n; i_1, \dots, i_k] = \frac{i_1 + \dots + i_k - i_1 \oplus \dots \oplus i_k}{n};$   $(ii) [n; i_1, \dots, i_k, j_1, \dots, j_t] = [n; j, j_1, \dots, j_t] + [n; i_1, \dots, i_k];$  $(iii) [n; i_1, \dots, i_k, j_1, \dots, j_t]$ 

$$= [n; j, s] + [n; i_1, \dots, i_k] + [n; j_1, \dots, j_t];$$
  
(*iv*) [n; *i*] = 0.

**Proof.** (*i*) Since  $j = i_1 \oplus ... \oplus i_k$ , it follows that  $i_1 + ... + i_k = tn + j$  for some  $t \in \mathbb{N}$ .

i.e.

ſ

$$\left[\frac{i_1+\ldots+i_k}{n}\right] = t = \frac{i_1+\ldots+i_k-j}{n},$$

$$n; i_1, \dots, i_k] = \frac{i_1 + \dots + i_k - i_1 \oplus \dots \oplus i_k}{n}.$$

(*ii*) Using (*i*) we obtain

$$=\frac{[n; j, j_1, \dots, j_t] + [n; i_1, \dots, i_k]}{j + j_1 + \dots + j_t - j \oplus s + i_1 + \dots + i_k - j}$$
$$=\frac{i_1 + \dots + i_k + j_1 + \dots + j_t - j \oplus s}{n}$$
$$= [n; i_1, \dots, i_k, j_1, \dots, j_t].$$

(*iii*) Follows from (*ii*). (*iv*) Follows from (*i*).

Applying Lemma 2.4, the condition (*ii*) in Theorem 1.1 can be written as

$$a_{i\oplus j} \le a_i + a_j + [n; i, j].$$

**Lemma 2.5.** Let  $G = [n; \{a_0 = 1, a_1, ..., a_{n-1}\}]$  be a numerical semigroup. Then for arbitrary  $i_1, ..., i_k \in \mathbb{Z}_n, k \in \mathbb{N}$  we have that

 $a_{i_1 \oplus \dots \oplus i_k} \le a_{i_1} + \dots + a_{i_k} + [n; i_1, \dots, i_k].$ 

**Proof.** The proof is by induction on k. It is easily seen that the inequality holds for k = 1. Namely,  $a_{i_1} =$ 

 $a_{i_1}$ . The condition (*ii*) in Theorem 1.1 implies that the inequality holds for k = 2. Assume that

 $a_{i_1 \oplus \dots \oplus i_k} \leq a_{i_1} + \dots + a_{i_k} + [n; i_1, \dots, i_k].$ The condition (*ii*) in Theorem 1.1, the inductive hypothesis and Lemma 2.4 imply that

 $\begin{aligned} a_{i_1 \oplus \dots \oplus i_k \oplus i_{k+1}} &\leq a_{i_1 \oplus \dots \oplus i_k} + a_{i_{k+1}} \\ + [n; i_1 \oplus \dots \oplus i_k, i_{k+1}] &\leq a_{i_1} + \dots + a_{i_k} + a_{i_{k+1}} \\ + [n; i_1, \dots, i_k] + [n; i_1 \oplus \dots \oplus i_k, i_{k+1}] \\ &= a_{i_1} + \dots + a_{i_k} + a_{i_{k+1}} + [n; i_1, \dots, i_k, i_{k+1}]. \blacksquare \end{aligned}$ For a numerical semigroup

 $G = [n; \{a_0 = 1, a_1, \dots, a_{n-1}\}]$ we define the following sets:

$$R(G) = \{i \oplus j | i, j \in \mathbb{Z}_n, a_{i \oplus j} = a_i + a_j + [n; i, j]\}$$
  
and  $S(G) = \mathbb{Z}_n \setminus R(G).$ 

Lemma 2.6.  $0 \in S(G)$ .

**Proof.** Since  $a_0, a_1, \dots, a_{n-1} \in \mathbb{N}$ , it follows that  $a_0 = 1 < a_i + a_j + [n; i, j]$  for all  $i, j \in \mathbb{Z}_n$ .

#### EMBEDING DIMENSION OF NUMERICAL SEMIGROUPS

We will give a characterization of the embedding dimension of numerical semigroups in the same manner as a characterization of the additive semigroups of integers was given in [1].

Let  $G = [n; \{a_0 = 1, a_1, \dots, a_{n-1}\}]$  be a numerical semigroup,  $B_0 = \{a_i n + i | i \in \mathbb{Z}_n\}$  and

 $\mathcal{M}_0 = \{a_i n + i | i \in R(G)\}.$ 

From the definition of  $B_0$  and  $\mathcal{M}_0$  it follows that  $|B_0 \setminus \mathcal{M}_0| = |\mathbb{Z}_n \setminus R(G)| = |S(G)|.$ 

**Theorem 3.1.** The set  $B_0 \setminus \mathcal{M}_0$  is the minimal set of generators for *G*. Thus,

 $ed(G) = |B_0 \setminus \mathcal{M}_0| = |S(G)|.$ 

**Proof.** We will consider the following four steps. Step 1. If  $R(G) = \emptyset$  then  $\mathcal{M}_0 = \emptyset$ . We will show that  $B_0$  is the minimal set of generators for *G* by contradiction.

Assume that, for some  $i \in \mathbb{Z}_n \setminus \{0\}$ ,

 $a_i n + i = a_{i_1} n + i_1 + \dots + a_{i_k} n + i_k$ , where  $k \ge 2$  and  $a_{i_s} n + i_s \in B_0 \setminus \{a_i n + i\}$  for each  $s \in \{1, \dots, k\}$ . Then

 $a_i n + i = (a_{i_1} + \dots + a_{i_k})n + i_1 + \dots + i_k$ 

 $= (a_{i_1} + \ldots + a_{i_k})n + [n; i_1, \ldots, i_k]n + i_1 \oplus \ldots \oplus i_k$ =  $(a_{i_1} + \ldots + a_{i_k} + [n; i_1, \ldots, i_k])n + i_1 \oplus \ldots \oplus i_k$ . This implies that  $i = i_1 \oplus \ldots \oplus i_k$  and

 $a_i = a_{i_1 \oplus \dots \oplus i_k} = a_{i_1} + \dots + a_{i_k} + [n; i_1, \dots, i_k].$ Let  $j = i_2 \oplus \dots \oplus i_k$  and assume that

 $a_i = a_{i_1 \oplus j} < a_{i_1} + a_j + [n; i_1, j].$  By Lemma 2.5 we have that

 $a_{i_1} + \ldots + a_{i_k} + [n; i_1, \ldots, i_k] = a_{i_1 \oplus \ldots \oplus i_k}$  $\leq a_{i_1} + \ldots + a_{i_k} + [n; i_1, \ldots, i_k].$  Next, the assumption and Lemma 2.5 imply that:

 $\begin{aligned} a_{i_1} + \dots + a_{i_k} + [n; i_1, \dots, i_k] &< a_{i_1} + a_j + [n; i_1, j] \\ &\leq a_{i_1} + a_{i_2} \dots + a_{i_k} + [n; i_2, \dots, i_k] + [n; i_1, j]. \end{aligned}$ This implies that

 $[n; i_1, \dots, i_k] < [n; i_2, \dots, i_k] + [n; i_1, j],$ contrary to Lemma 2.4 (*ii*).

Hence,  $a_i = a_{i_1} + a_j + [n; i_1, j]$ . So  $i \in R(G)$ , contrary to  $R(G) = \emptyset$ . Therefore,  $B_0$  is the minimal set of generators for *G*.

Step 2. Let  $R(G) \neq \emptyset$  and  $x_1$  be the largest element in  $B_0$  such that  $x_1 = a_{t_1}n + t_1$  and  $t_1 \in R(G)$ . This implies that  $t_1 = i \bigoplus j$  for some  $i, j \in \mathbb{Z}_n$  and  $a_{i \oplus i} = a_i + a_j + [n; i, j]$ .

Thus,

 $x_1 = (a_i + a_j + [n; i, j])n + i \oplus j$ =  $a_i n + a_j n + [n; i, j]n + i \oplus j$ =  $a_i n + a_j n + i + j = u + v$ ,

where  $u = a_i n + i$  and  $v = a_j n + j$ . Since u, v > 0, it follows that  $x_1 \neq u$  and  $x_1 \neq v$ . Therefore,

$$x_1 \in \langle B_0 \setminus \{x_1\} \rangle, \text{ i.e.}$$

 $\langle B_1 \rangle = \langle B_0 \rangle = G$ , where  $B_1 = B_0 \setminus \{x_1\}$ . If  $R(G) \setminus \{t_1\} = \emptyset$ , the same discussion as in Step 1, implies that  $B_1$  is the minimal set of generators for *G*. Step 3. We continue by induction to obtain the elements

 $t_1, \dots, t_r \in R(G), x_1 > x_2 > \dots > x_r \in B_0$ and  $B_r \subset B_{r-1} \subset \dots \subset B_1 \subset B_0$ , such that  $x_s = a_{t_s}n + t_s$  and  $B_s = B_{s-1} \setminus \{x_s\}$ , for every  $s \in \{1, \dots, r\}$ .

If  $R(G) \setminus \{t_1, ..., t_r\} = \emptyset$ , the same discussion as in Step 1, implies that  $B_r$  is the minimal set of generators for *G*. If  $R(G) \setminus \{t_1, ..., t_r\} \neq \emptyset$ , let  $x_{r+1}$  be the largest element in  $B_r$  such that  $x_{r+1} = a_t n + t$ for some  $t \in R(G) \setminus \{t_1, ..., t_r\}$ . This implies that  $x_r > x_{r+1}$  and  $a_t = a_{i \oplus j} = a_i + a_j + [n; i, j]$  for

some  $i, j \in \mathbb{Z}_n$ .

Thus,

$$x_{r+1} = (a_i + a_j + [n; i, j])n + i \oplus j$$
  
=  $a_i n + a_j n + [n; i, j]n + i \oplus j$   
=  $a_i n + a_j n + i + j = u + v$ ,

where  $u = a_i n + i$  and  $v = a_j n + j$ . From u, v > 0, we have that  $x_{r+1} \neq u$  and  $x_{r+1} \neq v$ .

Since  $x_1 > x_2 > ... > x_r > x_{r+1}$ , it follows that  $u, v \in B_0 \setminus \{x_1, ..., x_{r+1}\}$ , i.e.

 $x_{r+1} \in \langle B_{r+1} \rangle = \langle B_r \setminus \{x_{r+1}\} \rangle.$ Hence,

 $\langle B_{r+1} \rangle = \langle B_r \rangle = ... = \langle B_1 \rangle = \langle B_0 \rangle = G.$ Step 4. This procedure has to stop, since R(G) has a finite number of elements, i.e. there is some  $t_m$  such that  $R(G) \setminus \{t_1, ..., t_m\} = \emptyset$ . The same discussion as in Step 1 implies that  $B_m$  is the minimal set of generators for *G*. Since

 $|B_m| = |B_0 \setminus \{x_1, \dots, x_m\}| = |B_0 \setminus \mathcal{M}_0| = |S(G)|,$ we have

 $ed(G) = |B_0 \setminus \mathcal{M}_0| = |S(G)|.$ 

Let n be a given positive integer. Let  $T \subseteq$  $\mathbb{Z}_n \setminus \{0\}$  be a generating set for  $\mathbb{Z}_n$ , i.e.  $\langle T \rangle = \mathbb{Z}_n$ and let  $B(T) = \{b_s | s \in T\} \subseteq \mathbb{N}$  satisfies the following condition:

- if  $t \in T$  and  $t = i_1 \oplus \ldots \oplus i_r$  for  $i_1, \ldots, i_r \in T \setminus \{t\}$ ,
- then  $b_t < b_{i_1} + \ldots + b_{i_r} + [n; i_1, \ldots, i_r]$ . (1)
- We define a set  $P = \{a_0, a_1, \dots, a_{n-1}\}$  as follows: (*i*)  $a_0 = 1$ ;
- (*ii*) If  $i \in T$ , then  $a_i = b_i$ ;
- (*iii*) If  $i \notin T$ , then
  - $a_i = min\{b_{i_1} + \dots + b_{i_r} + [n; i_1, \dots, i_r]|i =$  $i_1 \oplus \ldots \oplus i_r, i_1, \ldots, i_r \in T$ .

By the definition of the set *P* it follows that for each  $i \in \mathbb{Z}_n \setminus \{0\}$ , there is  $t \in \mathbb{N}$  and some  $i_1, \ldots, i_t \in \mathbb{N}$ T such that

$$a_i = b_{i_1} + \ldots + b_{i_t} + [n; i_1, \ldots, i_t],$$
  
where  $i = i_1 \bigoplus \ldots \bigoplus i_t.$  (2)

**Theorem 3.2.** With the above notions, we have: (i) G = [n; P] is a numerical semigroup, denoted by [n; T; B(T)]. $(ii) R([n; T; B(T)]) = \mathbb{Z}_n \setminus (T \cup \{0\}).$ 

- (*iii*) ed([n; T; B(T)]) = |T| + 1.
- **Proof.**

(

(*i*) By (2) it follows that  

$$a_{i} = b_{i_{1}} + \dots + b_{i_{r}} + [n; i_{1}, \dots, i_{r}],$$

$$a_{j} = b_{j_{1}} + \dots + b_{j_{t}} + [n; j_{1}, \dots, j_{t}],$$
where  $i = i_{1} \oplus \dots \oplus i_{r}$  and  $j = j_{1} \oplus \dots \oplus j_{t}$  for some  
 $r, t \in \mathbb{N}.$   
If  $i \oplus j \in T$  then  

$$a_{i \oplus j} = b_{i \oplus j} < b_{i_{1}} + \dots + b_{i_{r}} + b_{j_{1}} + \dots + b_{j_{t}} + [n; i_{1}, \dots, i_{r}, j_{1}, \dots, j_{t}],$$
where  $i \oplus j = i_{1} \oplus \dots \oplus i_{r} \oplus j_{1} \oplus \dots \oplus j_{t}.$   
If  $i \oplus j \notin T$  then  

$$a_{i \oplus j} = \min\{b_{i_{1}} + \dots + b_{i_{k}} + [n; i_{1}, \dots, i_{k}]|i \oplus j$$

$$= i_{1} \oplus \dots \oplus i_{k}, i_{1}, \dots, i_{k} \in T\}$$

$$\leq b_{i_{1}} + \dots + b_{i_{r}} + b_{j_{1}} + \dots + b_{j_{t}} + [n; i_{1}, \dots, j_{t}].$$
In both cases, we have

$$\begin{aligned} a_{i\oplus j} &\leq b_{i_1} + \dots + b_{i_r} + b_{j_1} + \dots + b_{j_t} \\ &+ [n; i_1, \dots, i_r, j_1, \dots, j_t] \\ &= a_i - [n; i_1, \dots, i_r] + a_j - [n; j_1, \dots, j_t] \\ &+ [n; i_1, \dots, i_r, j_1, \dots, j_t] \\ &= a_i + a_j - [n; i_1, \dots, i_r] + [n; i_1, \dots, i_r, j] \\ &= a_i + a_j + [n; i, j], \end{aligned}$$

i.e.

$$a_{i\oplus j} \le a_i + a_j + [n; i, j].$$

Thus,  $a_0, a_1, \ldots, a_{n-1}$  satisfy the condition (*ii*) in Theorem 1.1 and G = [n, P] is a numerical semigroup.

(*ii*) Let  $t \in R(G)$ . Then  $t = i \oplus j$  and  $a_t = a_i + a_j + a_j$ [n; i, j], where

$$a_i = b_{i_1} + \ldots + b_{i_r} + [n; i_1, \ldots, i_r],$$
  

$$a_j = b_{j_1} + \ldots + b_{j_k} + [n; j_1, \ldots, j_k],$$
  

$$i = i_1 \bigoplus \ldots \bigoplus i_r \text{ and } j = j_1 \bigoplus \ldots \bigoplus j_k.$$

for  $r, k \in \mathbb{N}$ . If

$$t \in T \text{ then}$$

$$b_{i_1} + \dots + b_{i_r} + b_{j_1} + \dots + b_{j_k}$$

$$+[n; i_1, \dots, i_r, j_1, \dots, j_k]$$

$$> a_{i \oplus j} = a_t = a_i + a_j + [n; i, j]$$

$$= b_{i_1} + \dots + b_{i_r} + [n; i_1, \dots, i_r]$$

$$+ b_{j_1} + \dots + b_{j_k} + [n; j_1, \dots, j_k] + [n; i, j],$$
hich implies that
$$[n; i_1, \dots, i_r] + [n; j_1, \dots, j_k]$$

$$+[n; i, j] < [n; i_1, \dots, i_r, j_1, \dots, j_k],$$
  
v to Lemma 2.4. So  $t \notin T$ . This shows

contrary s that  $R(G) \subseteq \mathbb{Z}_n \backslash T.$ For t = 0,

$$a_0 = 1 < a_i + a_j + [n; i, j]$$
 for all  $i, j \in \mathbb{Z}_n$ , i.e.

 $t \in \mathbb{Z}_n \setminus (T \cup \{0\})$ . Hence,  $R(G) \subseteq \mathbb{Z}_n \setminus (T \cup \{0\})$ . Let  $t \in \mathbb{Z}_n \setminus (T \cup \{0\})$ . Since  $t \notin T \cup \{0\}$ , it follows that there are  $i_1, \ldots, i_r \in T$  and  $r \in \mathbb{N}$  such that

$$t = i_1 \oplus \ldots \oplus i_i$$

W

$$a_{t} = a_{i_{1} \oplus ... \oplus i_{r}} = b_{i_{1}} + ... + b_{i_{r}} + [n; i_{1}, ..., i_{r}]$$

$$= a_{i_{1}} + ... + a_{i_{r}} + [n; i_{1}, ..., i_{r}].$$
Let  $j = i_{2} \oplus ... \oplus i_{r}$ . Then
$$a_{t} = a_{i_{1}} + a_{i_{2}} + ... + a_{i_{r}} + [n; i_{1}, j] + [n; i_{2}, ..., i_{r}]$$

$$\geq a_{i_{1}} + a_{j} + [n; i_{1}, j] = a_{i_{1} \oplus j} = a_{t}.$$
Hence  $a_{i_{1}} = a_{i_{1}} + a_{i_{2}} + ... + a_{i_{r}} + [n; i_{1}, j] = a_{i_{1} \oplus j} = a_{t}.$ 

Hence  $a_t = a_{i_1} + a_j + [n; i_1, j]$ , which implies that  $t \in R(G)$ . This completes the proof, i.e.

$$R(G) = \mathbb{Z}_n \setminus (T \cup \{0\}).$$

(*iii*) Follows from (*i*) and (*ii*).

By all these results we obtain the following theorem: **Theorem 3.3.** A numerical semigroup G has ed(G) = d iff G = [n; T; B(T)] for some: positive integer n;  $T \subseteq \mathbb{Z}_n \setminus \{0\}$  such that  $\langle T \rangle = \mathbb{Z}_n$  and |T| = d - 1; and some  $B(T) \subseteq \mathbb{N}$ , that satisfies the condition (1).

#### FROBENIUS NUMBER OFNUMERICAL SEMIGROUPS

The Frobenius number F(G) of a numerical semigroup G is the largest integer not belonging to G. In fact, F(G) is the largest integer such that the linear equation  $m_1x_1 + \ldots + m_rx_r = F(G)$  does not have any non-negative integer solution, where

#### $\{m_1, ..., m_r\}$

is the minimal set of generators for G.

It is shown that if  $G = \langle m_1, m_2 \rangle$  and  $GCD(m_1, m_2) = 1$ , then  $F(G) = m_1m_2 - m_1 - m_2$  ([6]).

The question of finding a general formula for the Frobenius number, in terms of the minimal set of generators for *G* when  $ed(G) \ge 3$ , turned out to be much more difficult to answer.

F. Curtis has proved in [10] that Frobenius number cannot be given by "closed" formulas of a certain type when  $ed(G) \ge 3$ .

Several authors have developed algorithms that compute the Frobenius number of numerical semigroups with embedding dimension 3. The first is Johnson ([15]). Rødseth developed an algorithm using continued fractions ([14]). The algorithm by Davison ([16]) is the fastest known algorithm for computing the Frobenius number for ed(G) = 3, according to Beihoffer, Nijenhuis and Wagon ([17]).

Recently, an explicit general formula for computing F(G) for ed(G) = 3, was given by Denham in [18] and Tripathi in [19].

When ed(G) > 3, the Frobenius number has been exactly determined only for few special cases ([14]).

A variety of algorithms for computing the Frobenius number for ed(G) > 3, as well as upper bounds and lower bounds, are quite well elaborated in [14].

By Theorem 1.1, the Frobenius number of G = [n, A] is

$$F(G) = an + k - n,$$

where

 $a = max\{a_0, ..., a_{n-1}\}$  and  $k = max\{i|a_i = a\}$ . This is the simplest general form for the Frobenius number.

In continuation, we give a particular characterization of the Frobenius number of numerical semigroups with embedding dimension less than or equal to 3, in terms of its minimal set of generators.

Let 
$$G = [n; T; B(T)], T = \{j_1, \dots, j_k\},$$
  
 $\mathcal{A} = \{a_s n + s | s \in \mathbb{Z}_n\}$  and  
 $\mathcal{M} = \{b_{j_r} n + j_r | r = 1, \dots, k\},$  i.e.  
 $\mathcal{M} = \{m_1, \dots, m_k\}.$ 

We define  $\varphi: \mathbb{Z}^k \to \mathbb{Z}_n$  by

$$\varphi(z_1,\ldots,z_k) = t \text{ iff } \sum_{s=1}^k z_s m_s \equiv t \pmod{n}.$$

It is easy to check that the map  $\varphi$  is a homomorphism and  $H = \ker \varphi$  is an additive subgroup of  $\mathbb{Z}^k$  of rank *k*. Let  $B^0 = H \cap (\mathbb{N}_0)^k$ ,  $B = B^0 \setminus \{(0, \dots, 0)\}$ ,  $D = B + (\mathbb{N}_0)^k$  and  $C = (\mathbb{N}_0)^k \setminus D$ . (We say that *C* is the carrier of *G*).

**Theorem 4.1.** For each  $r \in \mathcal{A} \setminus \{0\}$ ,  $r = p_1 m_1 + \ldots + p_k m_k$  for some  $(p_1, \ldots, p_k) \in C$ . **Proof.** Assume contrary that for some  $r \in \mathcal{A} \setminus \{0\}$ ,  $r = p_1 m_1 + \ldots + p_k m_k$  and  $(p_1, \ldots, p_k) \notin C$ . Then  $(p_1, \ldots, p_k) \in B + (\mathbb{N}_0)^k$ , i.e.

$$(p_1, \dots, p_k) = (r_1, \dots, r_k) + (q_1, \dots, q_k) = (r_1 + q_1, \dots, r_k + q_k),$$

where  $(r_1, ..., r_k) \in B$  and  $(q_1, ..., q_k) \in (\mathbb{N}_0)^k$ . Since  $(r_1, ..., r_k) \in B$  it follows that

 $\varphi(r_1,\ldots,r_k)=0.$ 

This implies that  $\varphi(p_1, ..., p_k) = \varphi(q_1, ..., q_k)$ , and the obvious inequality

 $p_1m_1 + \ldots + p_km_k > q_1m_1 + \ldots + q_km_k$ contradicts the fact that  $r \in \mathcal{A} \setminus \{0\}$ .

If 
$$ed(G) = 1$$
 then  $T = \emptyset$  and  $G = \langle n \rangle$ . So,  
 $n = 1$  and the Frobenius number of G does not exist.  
Let  $ed(G) = 2$ , i.e.  $G = [n; \{i\}; \{b_i\}]$ , where

Let 
$$eu(G) = 2$$
, i.e.  $G = [n; \{l\}; \{b_i\}]$ , wher

 $GCD(n,i) = 1, \ x = b_i n + i, \ \mathcal{M} = \{x\} \text{ and } \\ \mathcal{A} = \{a_s n + s | s \in \mathbb{Z}_n\} = \{m_s | s \in \mathbb{Z}_n\}.$ 

The definition of G implies that  $m_{t\odot i} = tx$ , so the Frobenius number of  $G = [n; \{i\}; \{b_i\}]$  is

F(G) = (n-1)x - n = nx - x - n.Let ed(G) = 3, i.e.  $G = [n; \{i, j\}; \{b_i, b_j\}],$ 

where

$$GCD(n, i) = GCD(n, j) = 1, x = b_i n + i,$$
  

$$y = b_i n + i, \mathcal{M} = \{x, y\} \text{ and}$$

 $\mathcal{A} = \{a_s n + s | s \in \mathbb{Z}_n\} = \{m_s | s \in \mathbb{Z}_n\}.$ The definition of *G* implies that

 $m_s = \min\{px + qy | p \odot i \oplus q \odot j = s\}.$ 

If  $p' \odot i = q' \odot j$  and p' x > q' y, then

$$p' \odot i \oplus q \odot j = q' \odot j \oplus q \odot j = (q' + q) \odot j$$
  
and  $p'x + qy > (q + q')y$ .

Similarly, for 
$$p' \odot i = q' \odot j$$
 and  $q'y > p'x$ ,  
 $q' \odot j \oplus p \odot i = p' \odot i \oplus p \odot i = (p' + p) \odot i$   
and  $q'y + px > (p + p')x$ .

If  $p \odot i = q \odot j$ , then  $\varphi(p, -q) = 0$ , for the homomorphism  $\varphi: \mathbb{Z}^2 \to \mathbb{Z}_n$ , i.e.  $(p, -q) \in H$ . In order to find  $min\{px + qy\}$ , the above discussion shows that we have to have a good control on the pairs  $(p, -q) \in H$  for  $p, q \in \mathbb{Z}_n$ .

We say that a pair  $(p, -q) \in H$ , for  $p, q \in \mathbb{Z}_n$ , is a *minimal pair* if there is no  $(p', -q') \in H$ , for  $p', q' \in \mathbb{Z}_n$ , such that p' < p and q' < q. We say that two minimal pairs (p, -q), (u, -v) are *consecutive* if p > u, q < v and

 $0 < c < p, 0 < d < v \Rightarrow (c, -d) \notin H$ . We will prove the following lemma.

**Lemma 4.2.** Let (p, -q), (u, -v) be two minimal consecutive pairs. Then pv - qu = n and

 $\{s \odot i \oplus r \odot j | (s, r) \in A_L \cup A_R\} = \mathbb{Z}_n,$ where

$$A_{L} = \{(s, r) | 0 \le s < p, 0 \le r < v - q\}, A_{R} = \{(s, r) | 0 \le s 
Proof. Let
$$K = \{s \odot i \oplus r \odot i | (s, r) \in A_{L} \cup A_{R}\}.$$$$

The proof is in three steps.

Step 1. The assumption GCD(n, i) = GCD(n, j) = 1implies that for every  $t \in \mathbb{Z}_n$ ,  $t = \alpha \odot i \oplus \beta \odot j$  for some  $(\alpha, \beta) \in \mathbb{N} \times \mathbb{N}$ . If  $(\alpha, \beta) \in A_L \cup A_R$ , then  $t \in$ K. If  $(\alpha, \beta) \notin A_L \cup A_R$ , then we have to consider 4 cases:  $\alpha < p$ ,  $\beta < v$ ;  $\alpha \ge p$ ,  $\beta < v$ ;  $\alpha < p$ ,  $\beta \ge v$ ; and  $\alpha \geq p, \beta \geq v$ .

Case 1.  $\alpha < p, \beta < v$  and  $(\alpha, \beta) \notin A_L \cup A_R$ .

Since  $(\alpha, \beta) \notin A_L$ , it follows that  $\nu - q \leq \beta < \beta$ v, and since  $(\alpha, \beta) \notin A_R$ , it follows that  $p - u \leq \alpha$  $\alpha < p$ .

Next, the assumptions  $p \odot i = q \odot j$  and  $u \odot i = v \odot j$ imply that

 $(\alpha \ominus (p \ominus u)) \odot i \oplus (\beta \ominus (v \ominus q)) \odot j$  $= (\alpha - (p - u)) \odot i \oplus (\beta - (v - q)) \odot j$  $= \alpha \odot i \ominus p \odot i \oplus u \odot i \oplus \beta \odot j \ominus v \odot j \oplus q \odot j$  $= \alpha \odot i \oplus \beta \odot j = t = \alpha' \odot i \oplus \beta' \odot j,$ 

where

$$\alpha' = (\alpha - (p - u)) < \alpha < p \text{ and} \\ \beta' = (\beta - (v - q)) < \beta < v.$$

If  $(\alpha', \beta') \in A_L \cup A_R$ , then  $t \in K$ . If  $(\alpha', \beta') \notin$  $A_L \cup A_R$ , then we repeat the discussion above. After finitely many repetitions we will obtain that  $t \in K$ .

Case 2.  $\alpha \ge p, \beta < v$ .

If  $v - q \leq \beta < v$ , we apply the same argument as in Case 1, and obtain that  $t = \alpha' \odot i \oplus \beta' \odot j,$ 

where

 $\alpha' = (\alpha - (p - u)) < \alpha$  and  $\beta' = (\beta - (\nu - q)) < \beta < \nu.$ Next, let  $\beta < v - q < v$ . Then  $\beta + q < v \leq n$ , and  $(\alpha \ominus p) \odot i \oplus (\beta \oplus q) \odot j$  $= (\alpha - p) \odot i \oplus (\beta + q) \odot j$  $= \alpha \odot i \ominus p \odot i \oplus \beta \odot j \oplus q \odot j$  $= \alpha \odot i \oplus \beta \odot j = t = \alpha' \odot i \oplus \beta' \odot j,$ where

 $\alpha' = (\alpha - p) < \alpha$  and  $\beta < \beta' = (\beta + q) < v$ . In both cases, if  $(\alpha', \beta') \in A_L \cup A_R$ , then  $t \in K$ . Let  $(\alpha', \beta') \notin A_L \cup A_R$ . If  $(\alpha', \beta')$  is in Case 1, we obtain that  $t \in K$ . If  $(\alpha', \beta')$  is not in Case 1, then it is in Case 2, and we repeat the same discussion as above. After finitely many repetitions of the above discussion we will obtain that  $t \in K$ .

Case 3.  $\alpha < p, \beta \geq v$ . This case is symmetric to the Case 2. Case 4.  $\alpha \ge p, \beta \ge v$ .

By the same discussion as in Case 1, we obtain that  $t = \alpha' \odot i \oplus \beta' \odot j$ , where

$$\alpha' = (\alpha - (p - u)) < \alpha \text{ and} \\ \beta' = (\beta - (v - q)) < \beta.$$

If 
$$(\alpha', \beta') \in A_L \cup A_R$$
, then  $t \in K$ . If  $(\alpha', \beta') \notin A_L \cup A_R$ , we apply again one of the previous cases,

and after a finite number of such applications, we obtain that  $t \in K$ .

The above discussion implies that  $\mathbb{Z}_n \subseteq K$ . Step 2. Let  $(\alpha, \beta) \in A_R$  and  $(\alpha, \beta) \neq (0, 0)$ . Then  $0 < \alpha + u < p$  and  $0 < v - \beta < v$ . This, together with the assumption that (p, -q), (u, -v) are minimal consecutive pairs, implies that

 $(\alpha + u) \odot i \oplus (-(\nu - \beta)) \odot j \neq 0$ , i.e.  $(\alpha + u) \odot i \oplus (\beta - v) \odot j \neq 0.$ Since  $u \odot i \oplus (-v) \odot j = 0$ , we obtain that  $\alpha \odot i \oplus \beta \odot j \neq 0.$ Similarly, if  $(\alpha, \beta) \in A_L$  and  $(\alpha, \beta) \neq (0,0)$ , then  $\alpha \odot i \oplus \beta \odot j \neq 0.$ We have shown that for  $(\alpha, \beta) \in A_L \cup A_R$ ,  $\alpha \odot i \oplus \beta \odot j = 0 \implies (\alpha, \beta) = (0, 0).$ Step 3. Let  $(\alpha_1, \beta_1), (\alpha_2, \beta_2) \in K$  such that  $\alpha_1 \odot i \oplus \beta_1 \odot j = \alpha_2 \odot i \oplus \beta_2 \odot j$ , i.e.  $(\alpha_1 \ominus \alpha_2) \odot i \oplus (\beta_1 \ominus \beta_2) \odot j = 0.$ The conclusion of Step 2 implies that  $\alpha_1 \ominus \alpha_2 = 0$  and  $\beta_1 \ominus \beta_2 = 0$ , and since  $\alpha_1, \alpha_2, \beta_1, \beta_2 < n$  it follows that  $(\alpha_1,\beta_1)=(\alpha_2,\beta_2).$ 

Thus,  $K \subseteq \mathbb{Z}_n$ . This, together with Step 1, implies that  $K = \mathbb{Z}_n$ .

A simple calculation implies that

 $n = |K| = |A_L \cup A_R| = pv - qu$ .

Next, for  $G = [n; \{i, j\}; \{b_i, b_i\}, x = b_i n + i$ and  $y = b_i n + j$ , let:

-p be the smallest positive integer such that  $px > (p \odot i \odot j^{-1})y$ , and

- v be the smallest positive integer such that  $vv > (v \odot i \odot i^{-1})x.$ 

A simple calculation implies that the pairs

 $(p, -p \odot i \odot j^{-1})$  and  $(v \odot j \odot i^{-1}, -v)$  satisfy the condition of Lemma 4.2. Thus,

$$\mathcal{A} = \{sx + rv | (s, r) \in A_I \cup A_P\}$$
 and

$$F(G) = (n-1)x + (n-1)y$$

$$I(0) = (p - 1)x + (v - 1)y$$

 $-\min\{(v \odot j \odot i^{-1})x, (p \odot i \odot j^{-1})y\} - n.$ 

For a real number x, let [x] be the integer part of x, i.e. let [x] be the biggest integer smaller or equal than *x*, and let

$$[x] = \begin{cases} [x] + 1, & x \notin \mathbb{Z} \\ [x], & x \in \mathbb{Z} \end{cases}.$$

To find all the minimal pairs we start with the minimal pairs (n, 0) and  $(j \odot i^{-1}, -1)$ . The next minimal pair is  $\left(\left|\frac{n}{j\odot i^{-1}}\right|(j\odot i^{-1}) - n, -\left|\frac{n}{j\odot i^{-1}}\right|\right)$ . If (p, -q) and (u, -v) are two consecutive minimal pairs such that  $u \neq 0$ , then the next minimal pair is

$$\left(\left[\frac{p}{u}\right]u-p,-\left(\left[\frac{p}{u}\right]v-q\right)\right).$$

With the above discussion we proved the following theorem.

**Theorem 4.3.** Let  $G = \langle n, x, y \rangle$  be a numerical semigroup with ed(G) = 3. Then:

(*i*) There are unique  $p, q, u, v \in \mathbb{N}$  obtained by the procedure given above, such that:

$$px \equiv qy (mod n), vy \equiv ux (mod n),$$
  
$$px > qy \text{ and } vy > ux;$$

(*ii*) The Frobenius number F(G) of G is

$$px + vy - \frac{ux + qy - |ux - qy|}{2} - n - x - y. \blacksquare$$

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#### АДИТИВНИ ПОЛУГРУПИ ОД ЦЕЛИ БРОЕВИ. ДИМЕНЗИЈА НА НУМЕРИЧКИ ПОЛУГРУПИ

#### Виолета Анѓелкоска, Дончо Димовски

Факултет за информатика, Универзитет ФОН, Скопје, Република Северна Македонија Македонска академија на науките и уметностите, Скопје, Република Северна Македонија

Во овој труд дадена е карактеризација на димензијата на нумеричките полугрупи од аспект на структурата на адитивните полугрупи од цели броеви дадена во [1]. Дадена е експлицитна формула за Фробениусовиот број F(G) кога димензијата на нумеричката полугрупа G е помала или еднаква на 3.

Клучни зборови: нумерички полугрупи; димензија; Фробениусов број

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#### AN IMPRECISE PROBABILITY MODEL IN REPEATED INTERACTION GAMES

Nevena Serafimova <sup>1,\*</sup>, Dončo Dimovski<sup>2,\*</sup>

<sup>1</sup>Military Academy, University of Goce Delčev Štip, Skopje, Macedonia <sup>2</sup>Macedonian Academy of Sciences and Arts, Skopje, Macedonia <sup>\*</sup>e-mail: <u>nevena.serafimova@ugd.edu.mk; ddimovskid@gmail.com</u>

We introduce an imprecise probability model for general interaction games based on the Dirichlet family of multivariate probability distributions. In order to deal with the lack of evidence (ex-ante information), an ambiguity averse attitude of the players is incorporated into the payoff function. The existence of an ambiguity averse Nash equilibrium for the N – stage game is established as a classical result, composed of individual Nash equilibria for each separate round in the repeated game. The existence of a common belief about the probability distributions is an essential assumption for the analysis. In addition, further research directions are suggested.

Key words: game; interaction; imprecise probability; ambiguity aversion; Nash equilibrium

#### INTRODUCTION

Game theory is a mathematical approach to interactive decision-making. To participate in a game means to investigate and act, separately or jointly, to achieve the most favourable outcome, typically in uncertain and complex environments. Each player, acting in accordance to some rules and information structure, tries to maximize the personal gain expressed by some payoff function. Whether best options will be sought for depends upon numerous factors such as situation awareness, individual preferences, abilities, beliefs and their consistency, the level of confrontation etc. A successful game model should incorporate all relevant components into a single operational structure.

Games formalize interactions in many ways. In a population of players, there are different situations in which players' acts are intertwined. The characteristics of their interaction depend not only of the individual set of strategy and the payoff function, but also of the entire strategy profile of the population. Circumstances in which players are constrained to choosing a single action (or choose from a set of available actions) when interacting within a certain subset of players from the population, give rise to *local interaction games* [1]. A generalized class of interaction games was defined by Morris [2], of which local interaction games and other more specialized classes of games (such as games of incomplete information and random matching games), can be viewed as special cases. This generalization enables a unified approach in the analysis of the incorporated classes of games, as well as a new insight of the problems arising in different categories of models that can occur in these classes.

In an incomplete information game, players are uncertain about the environment that they are in. A player (or a type of players) is uncertain about the opposing player or type, which can be expressed by saying that each player is one of a large set of possible types, and the type profile for all players is drawn from some distribution. A player in a random matching game is uncertain about who the opponent is, while in local interaction games, the player faces a distribution over the actions of some nearby opponents. These three classes of games share the feature that each player (or player type) tends to choose an action that is a best response to a distribution of his opponents' actions [3].

In describing situations that reflect uncertainty about future events or outcomes, the classical prob-

abilistic models as defined by Kolmogorov are the usual choice. These models incorporate values which precisely estimate the uncertainty involved through an appropriate additive probability measure, without losing any information in the process. Mutually disjunctive elementary events are defined with probabilities expressed precisely by a number from the interval [0,1], with a request for unique previsions and conditional probabilities (for the non-zero probability events) to be determined. But in real decision situations, there is only limited information about probability distributions, which associates decision analysis with large uncertainty. It is very often the case that the probabilities of relevant events are ambiguous and precise values are impossible to define. Hence, the fulfillment of the requirements from the classical probability theory that arise from the additivity axiom is difficult and can lead to unavoidable measuring mistakes, incomplete statistical data, conflicting evidence and other problems, especially in situations where the factor of subjectivity is strong. As a result, the strict and highly demanding conditions of the classical probability calculus can not be considered appropriate for describing the problem when based on limited information.

To alleviate these difficulties, the precision requests concerning probabilities can be weakened to allow imprecise expression of individual probabilities. Imprecise probability is an extension and generalization of precise probability. Many concepts of precise probability theory can appropriately be generalized to imprecise probabilities, which express 'uncertainty about the uncertainty' or uncertainty of second order. These concepts allow overcoming the weaknesses of the traditional statistical approach and the often unmotivated assumptions for the applied functional forms of probability distributions. The imprecise probability models are needed in the inference processes when information is rare, unclear or conflicted, such is the situation in many real problems. In this sense, they can be considered as an essential step towards realistic decision making.

Game theory deals with the problem of uncertainty through applying the formal framework of Bayesian games. Still, its practical application is limited by the fact that quite often, the uncertainty is too complex to be adequately described by a classical, precise probability distribution. Simply applying tools from classical game theory to situations of complex uncertainty with only partial information about the current states of nature, could easily lead to wrong conclusions.

This paper presents a model for a particular class of games that are known as *interaction games*, as defined by Morris [2], with additional considerations

for the element of uncertainty about the states of nature that are expressed through a Bayesian imprecise probability model. The Bayesian approach usually assumes a prior Dirichlet distribution on the state space and makes inferences by conditioning the prior distribution to the observed data. One of the reasons for assuming a Dirichlet distribution is its computational simplicity, due to the fact that it is a conjugate density function to the multinomial distribution. Therefore, the posterior density will be also Dirichlet, with parameters updated according to the observations.

In addition, ambiguity aversion of players is assumed. An event is ambiguous when the player does not know its probability. Ambiguity aversion is simply a preference of the known over the unknown. Player's ambiguity attitude can be described upon defining a set of probability distributions over the set of all possible outcomes (states of the world). Then, ambiguity neutrality is expressed by indifference between all distribution mixtures in this set. Ambiguity aversion is exhibited if the player strictly prefers to restrict over some subset of these distributions. Conversely, the player exhibits a liking of ambiguity if strictly prefers the original distributions to some mixture over them.

The presented model is based on a repeated game structure, where a finite stage game is played multiple times (more precisely, there is a finite repetition of the same stage game). A usual convention holds - players know what all other agents did in the previous iterations, but have no knowledge of their moves in the current iteration. In this sense, it is an imperfect information game with perfect recall. The difference from classical models here is that the set of players with whom the interaction takes place, is not the same in each of the rounds. This issue is expressed by the payoff function, which is being adjusted according to the "evidence" i.e. the previous play.

The paper is organized as follows. Section 2 briefly describes the Dirichlet models of inference, presenting both the precise (PDM) and the imprecise (IDM) probability approach. The general interaction games of Morris are presented in Section 3. In Section 4, we present the model of Imprecise Probability Interaction Games (IPIG), by upgrading the interaction games with the elements from IDM. Some basic definitions are given and certain important issues are discussed. Finally, in Section 5 we conclude by discussing possible directions for further research.

#### THE IMPRECISE DIRICHLET MODEL IN A MULTIVALUE SAMPLING PROCESS

The power of the traditional probability theory to represent epistemic uncertainty has certain limitations. For example, the distributions that are used in probability models cannot recognize the situation of complete ignorance, when there is a total lack of information about the studied object or system. Such situations are usually described by applying uniform distributions, expecting that they will be further updated according to the new evidence. Still, the fact is that by introducing any form of distribution into the model, an extra knowledge has been added into the narrative.

Imprecision can result from many different circumstances, such as:

- not having enough data to determine a single prior belief;

- not being certain about the observation and measurement of data;

- the data are not specific (for example, when the observed data set is an unknown part of a bigger subset of the total state space);

- having several different opinions i.e. conflict or imprecision of the expertise;

- outliers or errors occurring in statistical sampling models, etc.

In this situations, imprecise probabilities (initial work by Walley, Fine, Kuznetsov) are defined as models for behaviour under uncertainty that correspond, in general, to a set of probability distributions. The theory that deals with imprecise probabilities is completely based on classical probability. As a generic term, imprecise probability refers to all mathematical models, both qualitative (imprecise) and quantitative (non-additive), that are not using sharp numerical measures for probability.

There are many ways in which imprecision can be expressed. Among them are probability intervals, sets of probability measures, lower and upper previsions, credal sets, belief functions, convex capacities, fuzzy measures. Although it might seem differently, all these models can be expressed in an equivalent manner by using lower and upper previsions. Thus, the theory of lower and upper previsions, introduced by Walley [4], provides the most general framework for incorporating imprecision in the models of decision-making.

The lack of information can be overcome by applying the Imprecise Dirichlet Model (IDM). Instead of a single density, IDM considers a set of prior densities on the parameter space. Having a set of densities instead of only one, the mathematical expectation for a measurable and bounded function with respect to all densities from this set will not be a single value, but a pair of lower an upper provisions, obtained by considering infimum and supremum values over the prior's set. It should be noted that the IDM model allows coverage not only of lack of evidence but is also suitable for cases where conflicting information from different sources exists [5].

First, let's investigate the Precise Dirichlet Model (PDM). The use of Dirichlet distribution in probability updating models is very appropriate because, next to the fact that the set of these distributions is very rich, any prior distribution can be approximated by a finite mixture of Dirichlet distributions. An important statistical property of PDM is that the density functions constitute a conjugate family with respect to multinomial likelihoods: if the prior is Dirichlet, the posterior distribution will also be a Dirichlet probability distribution.

To formulate PDM, we observe N realizations of the *m* possible states  $\omega_i$  from the state space  $\Omega = \{\omega_1, \dots, \omega_m\}$  according to the standard multinomial model. The probabilities for occurrence of each of the states from  $\Omega$  are formalized as follows:

$$P(\omega_i) = \Theta_i, \ \Theta_i \ge 0 \text{ and } \sum_{i=1}^m \Theta_i = 1.$$

By defining  $n_i$  to be the number of observations of the state  $\omega_i$  in N trials, we can construct a vector of random variables  $n = (n_1, \dots, n_m)$ ,  $\sum_{j=1}^{m} n_j = N$ . In the PDM with parameters *s* and  $(t_1, \dots, t_m)$ , the prior probability distribution for  $\theta = (\theta_1, \dots, \theta_m)$  is given by the density function:

$$p(\theta) = \Gamma(s) \cdot \frac{\prod_{i=1}^{m} \theta_i^{st_i - 1}}{\prod_{i=1}^{m} \Gamma(st_i)}$$

where  $\Gamma$  is the Gamma-function. The posterior distribution is given by the density function:

$$p\left( \theta \left| n 
ight) \propto \prod_{i=1}^{m} \theta_{i}^{n_{i}+st_{i}-1}$$
 .

which is also a Dirichlet distribution when multiplied by the multinomial likelihood function relative to n, with updated parameters N+s and  $t^* = (t_1^*, \dots, t_m^*)$ , where  $t_i^* = (n_i + st_i)/(N+s)$ .

The hyper-parameter s > 0 in the PDM determines the influence of the prior over the posterior distribution: the bigger its value, the greater is the uncertainty about the observations and consequently, the convergence of the upper and lower probabilities will be slower, and the conclusions should be more cautious. The value of this parameter should not depend on the number *m* of all possible states of

nature or the total number N of observations. Walley [4] has defined *s* as the number of observations that will reduce the difference between upper and lower probabilities to half of its initial value. Smaller values of *s* will signify faster convergence with increased precision of the conclusions, while for large values of *s* the conclusions will be weaker. Some authors adopt different value ranges for *s*, for example: s > 0, s > 1,  $s \in [1,2]$  etc.

Each of the  $t_i$  is the mean value of the respective  $\theta_i$ . In order to reliably choose a fixed value for  $t_i$ , the experimental evidence should be extensive i.e. the value of N should be high. There are many situations where this is not possible. The alternative approach is to switch to the Imprecise Dirichlet Model (IDM), which takes into consideration all possible values for  $t_i \in (0,1)$  i.e. the entire interior of the m-

dimensional unit simplex  $\Delta^m$ .

Now, if n(A) is the number of observations of the subset A of  $\Omega$ , then the predictive probability P(A,s) of A with the Dirichlet prior from PDM, relative to N, will be given as:

$$P(A \mid s, t, n) = \frac{n(A) + s \cdot t(A)}{N + s}, \text{ where}$$
$$t(A) = \sum_{\omega_i \in A} t_i.$$

This probability value can be maximized and minimized over  $(t_1, \ldots, t_m) \in \Delta^m$ , in order to obtain the posterior lower and upper predictive probabilities of *A*:

$$\underline{P}(A/n,s) = \frac{n(A)}{N+s},$$
$$\overline{P}(A/n,s) = \frac{n(A)+s}{N+s}$$

Hence, the probability for occurrence of some element (state) from A, will be a number from the interval between these two values. If it is not certain which of the states  $\omega_i \in A$  have been observed, the lower and the upper bounds for the probability of A can still be estimated, taking into account all possible k = 1, ..., M subsets of the state space  $\Omega$  and all  $(t_1, ..., t_m) \in Int\Delta^m$  from the interior of the m-dimensional unit simplex  $\Delta^m$ :

$$\underline{P}(A,s) = \min_{k} \inf_{t} \frac{n^{(k)}(A) + s \cdot t(A)}{N+s}$$

$$\overline{P}(A, s) = \max_{k} \sup_{t} \frac{n^{(k)}(A) + s \cdot t(A)}{N + s}.$$
  
Clearly,  $n^{(k)}(A) = \sum_{\omega_{i} \in A} n^{(k)}_{i}$ , where  $n^{(k)}(A)$ 

is the number of observations of the enumerated combination of states k. The infimum value of t(A) is 0 and the supremum is 1 for all  $A \neq \Omega$ , while for  $A = \Omega$  we have a unique value t(A) = 1.

For considering the minimum and the maximum of  $n^{(k)}(A)$ , we divide the power set of  $\Omega$  in three parts: the family  $F_1$  of subsets of A, the family  $F_2$  of sets B such that  $B \cap A = \emptyset$  and the family  $F_3$ of sets that do not belong to  $F_1 \cup F_2$ . Then, setting  $c_i$  to be the number of occurrences of the set  $A_i$ , we have:

$$\min_{\substack{k=1,\dots,M}} n^{(k)}(A) = \sum_{A_i \in F_1} c_i, \text{ and}$$
$$\max_{\substack{k=1,\dots,M}} n^{(k)}(A) = N - \sum_{A_i \in F_2} c_i = \sum_{A_i \cap A \neq \emptyset} c_i.$$

Choosing an interval in order to present imprecision of knowledge or observations is suitable for several reasons. Statistical distributions need assumptions of distribution types, distribution parameters and a mapping from events to real values between 0 and 1. Fuzzy sets need assumptions of not only lower and upper bounds, but also membership functions. The interval on the other hand is presented in a simple form, by a pair of numbers (the lower and the upper bound), is easily understandable and does not assume any kind of distribution. Given that the essence of epistemic uncertainty is the lack of knowledge, a representation with the least assumption is the most desirable.

#### INTERACTION GAMES

When a large population of players interacts strategically, some encounters may be more likely to happen than others. From a game – theoretical perspective, this situation becomes interesting when it is assumed that the player cannot decide separately for each possible encounter (group of interacting players), but instead must choose a fixed strategy that will be played against all of them. This situation should not be confused for incomplete information

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in games, which is a canonical way of modelling strategic environments in the presence of uncertainty about players' preferences, their beliefs about other player' beliefs about preferences, and so on. In interaction games, large populations of players interact strategically without uncertainty, but dealing only with subsets of the total population.

The generalized interaction games have been defined by Morris [3]. They include a finite or a countably infinite population of players, each of which participates in a game with a random group (a subset) of other players. The convention in game theory is that the individual payoffs of all players depend on the strategic profile of the entire population – in this case, of the group of participating players. Interaction games have two more conventions:

(i) in each of the repeated encounters, the player should choose the same strategy, and

(ii) the final payoff will not depend on the strategies of the non-participating players.

Interactions have weights, and the equilibrium of the interaction game is a strategic profile that enables each player to maximize the weighted sum of payoffs from each interaction. The definition of the equilibrium in general interaction games corresponds to the standard Nash Equilibrium in games with incomplete information [2].

Below we briefly present the formal model of general interaction games.

A population X of players is observed, which is finite or possibly countably infinite. For each player  $x \in X$ , a set  $A_x$  of actions (pure strategies)  $a_x$ of x for the standard strategic form game is given, and a payoff function  $u_x : A \to \mathbf{R}$  is defined over the product space  $A = \bigotimes_{x \in X} A_x$ . The individual mixed strategies  $\alpha_x$  of x are defined by probability distributions over  $A_x$  i.e.  $\alpha_x \in \Delta A_x$ . If the strategic set  $A_x$  is infinite, then it is agreed that the mixed strategies should have a finite support. Mixed strategy profiles that include all players can be represented by vectors  $\alpha \equiv {\alpha_x}_{x \in X}$ .

In the interaction game, each player can be involved with a random group of other players. The possible interaction groups are described by a set Iof subsets from X (elements of the power set  $2^X$ ), such that the elements of an arbitrary set from I are the participating players in a single (one shot) game. The elements of I are called *interactions*. In addition,  $I_x$  denotes the set of interactions of the player  $x \in X$ ,

$$I_x = \left\{ Q \mid Q \in I, x \in Q \right\}.$$

Clearly,  $I = \bigcup_{x \in X} I_x$ . It can be agreed that the cardinality of all elements of I is not less than 2, in order to exclude the degenerate cases of the 'zero player' games and games with only one player, which is a classical case of decision-making. Further on, we will denote pure and mixed strategies that are played within an interaction Q by (a, Q) and  $(\alpha, Q)$  respectively.

The likelihood of a particular interaction to effectuate is defined by a weight function  $P: I \rightarrow \mathbf{R}^+$ , such that for all  $x \in X$  it holds that  $0 < \sum_{Q \in I_X} P(Q) < \infty$ . The last condition ensures that

each player will participate in at least one interaction, but also that the total participation of the player in different interactions will be bounded.

Now, the pure strategy payoff for the player x can be defined as a weighted sum of the payoffs  $u_x$  from the individual interactions, depending on the chosen pure strategy a:

$$v_x(a): A = \bigotimes_{x \in X} A_x \to \mathbf{R}$$
, defined by  
 $v_x(a) = \sum_{Q \in I_x} P(Q) u_x(a,Q)$ .

For the latest sum to be well defined, it is assumed that the payoffs  $u_x(a,Q)$  are bounded for all x. Similarly, the payoff that x receives from a mixed strategies profile  $\alpha$  that was played in the interaction Q, can be defined as:

$$v_x(\alpha) = \sum_{Q \in I_x} P(Q) u_x(\alpha, Q), \text{ where}$$
$$u_x(\alpha_Q, Q) = \sum_{a_x} \left( \prod_{y \in X} \alpha_y(a_y) \right) u_x(\alpha, Q).$$

The general class of interaction games allows a unified representation of several other classes (such as incomplete information, local interaction and random matching games), by capturing their common structural elements. A dynamic interpretation of the model with continuum of players, has also been formulated and discussed [3]. The common structure of interaction games helps in better understanding each of the separate classes of games.

#### THE PROPOSED MODEL

In this section, we define the imprecise probability model of a repeated interaction game, by in-

troducing Walley's formulation into the general class of interaction games as defined by Morris. A repeated game is an extensive form game that consists of a number of repetitions of some base game, called *stage game*. Thus, the stage game is a normal (one shot) game in which players act simultaneously. In the proposed model, each player chooses a strategy, while repeatedly faced with uncertainty about the set of participating players (opponents) that are involved in the interaction. The uncertainty comes from not having ex-ante information about the group of players (a subset of the total set of players that participate in the game) that will interact in the next stage. In response to this situation, the states of nature are presented by the interaction subsets of players and the IDM model is applied to express the uncertainty.

**Definition 1.** The model of an Imprecise Probability Interaction Game (IPIG) consists of:

i. a set of players X;

ii. a set of pure strategy profiles  $A = \bigotimes_{x \in X} A_x$ ;

iii. a payoff function  $v = \{v_x\}_{x \in X}$  defined on

iv. a finite set of interactions

 $I = \{Q_i \mid j = 1, ..., m\}$  (the state space);

v. an imprecision parameter s.

In addition, we make some structural assumptions and clarifications.

A1. Each player x interacts within sets of players. The set of all interactions of x is denoted by  $I_x$  and it is a subset of I.

A2. The sets X, A and I and the payoff v are common knowledge.

A3. The players are not sure about the interaction they will be involved in.

A4. The total payoff received by a player x is the sum of the payoffs from each of the previously participated interactions.

A5. At each stage, only one interaction from I can take place.

With the above settings, the IPIG model is a tuple (X, A, v, I, s) representing an upgrade of the general interaction game that incorporates uncertainty. The individual mixed strategies are defined in the usual way, as are the combined profiles of pure and mixed strategies.

Let's suppose that there are total of *m* interaction groups, card(I) = m, and that the elements (interactions)  $Q_j$  (j = 1, ..., *m*) from *I* are appropriately indexed. Since the probability of a player *x* to ob-

serve a particular interaction  $Q \in I_x$  is imprecise, the payoff function cannot be deterministically formulated. Instead, we will define lower and upper limits of the expected payoff, using the previously discussed IDM.

**Definition 2.** For a mixed strategy  $\alpha$ , the total expected payoff of player *x* with respect to the probability distributions over the interaction's set *I* is the weighted sum of the payoffs from all interactions of *x* when  $\alpha$  is played, integrated over the distribution space  $\Delta^m$ :

$$Ev_x(\alpha) = \int_{\pi \in \Delta^m} \sum_{j=1}^m \left( v_x(\alpha, Q_j) \cdot \pi_j \right) p(\pi) \, d\pi \, .$$

Here  $\pi$  has the precise multinomial Dirichlet distribution over *I*,  $\pi_j$  is the probability of  $Q_j$  according to  $\pi$ , and  $v_x(\alpha, Q_j)$  denotes the payoff of *x* from an engagement in the interaction  $Q_j$  when the strategy profile  $\alpha$  was observed.

The subjective probability p over the unit simplex  $\Delta_I$  (a second-order probability over I) expresses the ambiguous attitude of the player, i.e. the subjective uncertainty about the "true" probability  $\pi$ . We have:

$$Ev_{x}(\alpha) = \sum_{j=1}^{m} v_{x}(\alpha, Q_{j}) \int_{\pi \in \Delta^{m}} \pi_{j} p(\pi) d\pi =$$
$$= \sum_{j=1}^{m} v_{x}(\alpha, Q_{j}) E_{p} \pi_{j}$$

where  $E_p \pi_j$  is the expected value of  $\pi_j$  in respect to the probability *p* that the particular distribution  $\pi$ , of which  $\pi_j$  is a component, will be observed.

According to the pervious discussions related to the lack of evidence, the expected value for the probability  $\pi_i$  for observing  $Q_i$  with respect of

 $p(\pi)$  can be estimated by  $E_p \pi_j = \frac{n_j + st_j}{N + s}$ , which leads to the following expression:

$$Ev_{x}(\alpha) = \sum_{j=1}^{m} v_{x}(\alpha, Q_{j}) \cdot \frac{n_{j} + st_{j}}{N + s}.$$
 (1)

The ambiguity about the parameters that are applied in (1) imposes payoff concerns and motivates an ambiguity averse approach in search for a possible strategic advantage, when faced with the uncertain interaction set. As before, for the purpose of eliminating the hyper-parameter t, we introduce

A;

intervals for the expected payoff  $v_x(\alpha)$  by accounting all values of  $(t_1, \ldots, t_m) \in \Delta^m$  in (1):

$$\underline{\underline{E}} v_x(\alpha) = \inf_{t \in \Delta^m} E v_x(\alpha) ,$$
$$\overline{\underline{E}} v_x(\alpha) = \sup_{t \in \Delta^m} E v_x(\alpha) .$$

Consequently, the payoff function  $v_x$  of x will be presented as an interval:

$$\left[\underline{E}v_x(\alpha), \overline{E}v_x(\alpha)\right].$$

The interval-valued expected payoffs can be compared according to different criteria. Among them are: the criterion of maximality, the concept of admissibility, the ambiguity aversion approach etc. In order to define a solution concept for a game, a specific criterion should be chosen. Here, we refer to the pessimistic (lower limit) payoff evaluation and define the strict ambiguity aversion under the previously described circumstances. Ambiguity averse behavior is often viewed as a robust response to doubts about beliefs. Under strict ambiguity aversion every strategy is evaluated by its minimal expected payoff, allowing the interval-valued expectations to be replaced by the correspondent lower interval limits.

In defining the expected ambiguity averse payoff for a given mixed strategy, we follow a representation approach given in [7].

**Definition 3.** The player x's payoff under a mixed strategy profile  $\alpha$  and strict ambiguity aversion in a repeated game is defined as:

$$V_{\alpha,x} = \frac{s}{N+s} \cdot V_0 + \sum_{k=1}^m \frac{c_k}{N+s} \cdot V_k , \quad (2)$$

where *N* is the number of stage games in the repeated game,  $c_k$  is the number of occurrences of the interaction  $Q_k$ ,  $V_i = \min_{j \in \Delta^m} v_x(\alpha, Q_j)$  for i = 1, ..., n, and  $V_0 = \min_{j=1,...,m} v_x(\alpha, Q_j)$ .

This definition takes into account all payoffs from previous stage games, thus it is history-related and involves an element of learning.

Next, we define a Nash equilibrium solution concept for a repeated imprecise interaction game under strict ambiguity aversion. This definition implicitly involves an updating assumption that takes into consideration the observed play and the received payoffs from the previous stage games. It should be noted here that the described situation differs from the standard repeated game model, where the stage game is always the same and consequently, the circumstances supporting a Nash equilibrium play remain invariable. In our model, the situation changes with the history since interactions may vary, with the results from these changing interactions of the previous rounds being incorporated into the payoff function.

**Definition 4.** The strategy profile  $\alpha^* \in \Delta A$  is *an ambiguity averse Nash equilibrium* of a stage game in the imprecise probability interaction game (X, A, v, I, s), if for all  $x \in X$  and all mixed strategy profiles  $\alpha \in \Delta A$ , it holds that:

$$V_{\alpha^*, x} \geq V_{(\alpha^*_{-\chi}, \alpha_{\chi}), x}$$
.

Here,  $\alpha_{-x}^*$  denotes the opponents' strategy profile for the player x within the strategy profile  $\alpha^*$ , while  $\alpha_x$  is an arbitrary strategy of x. The equilibrium definition requires that given the expected payoff (2), each of the players best responds to the strategies of all other players in the game. To the extent that there is a lack of evidence to precisely define the Dirichlet prior over the state space, the ambiguity related to its parameters translates into ambiguity about the equilibrium play. By applying ambiguity aversion to the parameter t (more precisely, a pessimistic approach by endorsing minimum payoff values) the payoff function (2) incorporates only one parameter - namely s, whose value in general may not be shared by all players. In case there is a common belief about the value of s, the defining solution of each separate stage game will coincide with a classical Nash equilibrium of a normal form game. We will formalize this discussion in the following theorem.

**Theorem.** Let G be a repeated game for the finite imprecise probability interaction game (X, A, v, I, s) with finite population of players. If for the first N rounds in G, there is a common belief about the value of the parameter s of the Dirichlet prior over the set of all possible interactions, then there exists a (mixed) ambiguity averse Nash equilibrium for G in the N - stage game and it is a Nash equilibrium sequence of ambiguity averse Nash equilibriums from each of the first N rounds.

The idea underlying this theorem and its proof comes directly from the classical result for equilibria existence in (complete information) finite strategic form games. Having that any sequence of stagegame Nash equilibria is a subgame-perfect equilibrium (SPE) in a finite repeated-game (i.e. it is a Nash equilibrium in every subgame of the original game) [8], this theorem also ensures the existence of a SPE in this model of imprecise probability interaction games. The existence of a common belief about the probability distributions is an essential assumption for the analysis. Depending on the beliefs that players hold for the unknown elements (probability distributions, parameters), ambiguity aversion may expand, shrink or simply change the equilibrium set. Holding payoffs and the structure of the underlying game fixed, ambiguity aversion may expand the set of equilibria relative to the groups that share a common belief about distributions. Without this restriction (i.e. taking into account all possible distributions), ambiguity aversion will not affect the equilibrium set [6].

As previously discussed, it is not necessary for the value of the parameter *s* to be identical for all players, as long as its individual estimations are common knowledge. Alternatively, if this is not the case i.e. players have private estimations for s that are not publicly known, a Bayesian game can be considered where a player could analyze the game conditioning on various players' types, where the prior probability distribution over types is assumed to be common knowledge. When appropriate, this can be presented by enlarging the interaction set I in the game model. The result would be a Bayesian (Nash) equilibrium (BNE), a straightforward extension of the Nash equilibrium which depicts the uncertainty about the parameters and the way in which players react to that uncertainty. In BNE, each type of player chooses a strategy that maximizes expected utility given the actions of all types of other players and their beliefs about other players' types.

#### FURTHER RESEARCH CONSIDERATIONS

In this paper, we have introduced an imprecise Dirichlet model for general interaction games. In order to deal with the lack of evidence (ex-ante information), an ambiguity averse attitude of the players is incorporated into the payoff function. This approach ensures the existence of a (sequential) Nash equilibrium for the N – stage game, composed of individual Nash equilibria for each separate round. In essence, being a combination of changing interactions, uncertainty and ambiguity, the model raises many research questions.

There are various directions in which the analysis of this game model can unfold, each referring to different issues and considerations. To begin with, ambiguity, unlike fundamental uncertainty, may disappear with the passage of time simply because the increasing evidence will provide means for improved estimation of the unknowns, in this case the parameters of the applied IDM. While considering new evidence, the strict ambiguity criterion that is applied to game payoffs can easily prove to be over-pessimistic. For this reason, more sophisticated representations of the interval-valued expected payoffs that consider players' attitude towards ambiguity are desirable.

Possible modifications of the model can account for different payoff functions that depart from the ambiguity – averse standpoint or are adjusted to an infinite repeated game model that incorporates a discount factor. Another obvious possibility is to consider a replacement of the imprecise Dirichlet model with a different type of uncertainty presentation such as, for example, belief functions of the Dempster – Shafer theory of evidence. The later is actually a generalization of probability theory which, by assigning probability to sets (of events) instead of singletons, enables a more abstract approach towards evidence at hand. Moreover, if the available evidence permits assignment of precise probabilities to single events, the Dempster - Shafer theory will seize down to the traditional probabilistic model.

The proposed model may be analyzed more in detail in reference to subfamilies of the generalized interaction games, such as random matching games or local interaction games. The influence of the parameter s on the equilibrium behavior could be another point of interest. Finally, complementing the assumption of ambiguity aversion with the assumption of dynamic consistency, which can lead to equilibrium sets of games with ambiguity averse players coinciding with the equilibrium sets of Bayesian games [9], can also be considered.

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#### МОДЕЛ НА НЕПРЕЦИЗНА ВЕРОЈАТНОСТ ВО ПОВТОРЕНИ ИГРИ НА ИНТЕРАКЦИЈА

#### Невена Серафимова<sup>1,\*</sup>, Дончо Димовски<sup>2,\*</sup>

## <sup>1</sup>Воена академија, Универзитет "Гоце Делчев", Штип, Скопје, Република Македонија <sup>2</sup>Македонска академија нанауките и уметностите, Скопје, Република Македонија

Воведуваме модел на непрецизна веројатност кај општите игри на интеракција, врз основа на фамилија мултиваријантни распределби на веројатност на Дирихле. Притоа, отсуството на претходна информација е искажано преку аверзија кон повеќезначност кај играчите, која е вградена во функцијата на добивка. Дефиниран е Нешов еквилибриум со аверзија кон повеќезначност во повторената игра на интеракција, кој се состои од Нешови еквилибриуми на секоја од рундите и утврдено е неговото постоење, врз основа на класичната теорија. Клучна претпоставка во анализата е општото верување за распределбите на веројатност во моделот на Дирихле. На крајот, дадени се насоки за идни истражувања.

**Клучни зборови:** игра; интеракција; непрецизна веројатност; аверзија кон повеќезначност; Нешов еквилибриум

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