Towards a Knowledge Graph for the Visual Recognition of Skin Cancer

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***Abstract*—The evolution of Knowledge Graphs (KGs), during the last two decades, has encouraged developers to create more and more context related KGs. This advance is extremely important because Artificial Intelligence (AI) applications can access open domain specific information in a semantically rich, machine understandable format. In this paper, we present a KG for the various types of Skin Cancer, which can represent information about the symptoms and dangers to provoke, of the most common, based on cases, types of Skin Cancer. Moreover, we provide a data integration mechanism that can map information from various datasets with skin cancer cases into the skin cancer ontology. A use case scenario in which the KG can be used as a decision support system by doctors, is provided, in which a Computer Vision (CV) simulates a doctor. The CV mechanism in the cases that is not able to classify the case it can consult the KG to retrieve similar cases based on the characteristics of the one at hand.**

***Index Terms*—Knowledge Graph, Data Integration, Computer Vision, Decision Support System, Skin Cancer**

I. Introduction

The creation of context related Knowledge Graphs (KGs), i.e., KGs that can be used only in specific environments, seems to be the next step for allowing KGs to become the main knowledge representation format for the Web [1]. Our focus in this work is on representing information about the most common types of *skin cancer*, based on cases, which in this case are the *basal cell carcinoma* (bcc), *squamous cell carcinoma* (scc), and *melanoma* (mel), following the official statistics of the World Cancer Research Fund[1]. More specifically, the KG can represent information about the symptoms of the three aforementioned types, dangers that increase the risk to provoke one of the aforementioned skin cancers, information about the family history of each patient, and body characteristics. For this reason, we also provide a mechanism that can integrate the data from the various data sources of the KG along with their metadata (i.e., symptoms, patient characteristics, etc). Moreover, we provide an information retrieval mechanism based on a set of competency questions (i.e., questions that we as users would like the KG to able to answer), which was gathered by doctors. These competency questions are basically the most common questions that doctors or patients ask about a specific case which might (or not) be skin cancer, such as *"Which are the symptoms for melanoma?"*, *"Which are the dangers which increase the risks to provoke a squamous cell carcinoma?"*, among others.

The Skin Cancer KG was developed in order to assist doctors in general, over their diagnosis of potential skin cancer cases. In other words, the KG is set to help doctors as a decision support system in potential skin cancer cases that they are uncertain weather it is a positive or negative case, before moving to a biopsy. The Skin Cancer KG will return similar images of positive cases based on the characteristics that they have for the case at hand. Moreover, it will return characteristics for the people that suffered from a skin cancer case, such as the skin type, age, gender, body type (e.g., percentage of fat), family and personal history, state of immune system, and what the patient has been exposed to (e.g., sun, radiation, etc).

To simulate a use case scenario we use a Computer Vision (CV) mechanism that acts as a doctor in this case that fails to recognize a potential skin cancer case. The CV mechanism is trained on the Skin Cancer MNIST: HAM10000 [2], and then is tested with some completely new images of skin cancer cases extracted from [3]. Therefore, when the CV is uncertain of classifying a specific image in a type of skin cancer, in our case bcc, scc, and mel, the information retrieval mechanism that we have developed will retrieve from the KG similar cases of skin cancer based on the characteristics of the image that the CV is uncertain to classify. For instance, if the image that the CV tries to classify has specific colour, an asymmetric diameter, is bleeding, and has a bump, the information retrieval mechanism will return all of the skin cancer cases with exactly the same characteristics. The user can apply various restrictions on the returned results, for example the cases which are displayed to be only from males or females.

Our contribution in this paper, is on one hand the Skin Cancer KG which can represent information about various type of skin cancer and the dangers that can provoke them, which in turn can be used by doctors, in order to take a decision

[1] https://www.wcrf.org/cancer-trends/skin-cancer-statistics/

before moving to a biopsy. Moreover, the paper presents a data integration mechanism which translates information from skin cancer datasets into instances of the KG. We also provide an information retrieval mechanism that returns crucial information for the characteristics of the bcc, scc, mel skin cancer types, the dangers that provoke them, and the patient characteristics.

The rest of this paper is organized as follows. Section II, discusses the related work. Next, in Section III we present the Skin Cancer KG, the Data Integration mechanism which maps the data into the ontology of the KG, the Information Retrieval mechanism, and we also describe the architecture of the CV mechanism. Section IV, describes the use case scenario that we analyzed. Section V, contains the evaluation of the KG and the CV mechanism, and we conclude our paper with Section VI.

II. Related Work

The area of KGs for Medical Informatics is quite rich and many studies have been presented, which establishes the area of Medical Informatics as one which has the most KGs, in regards of quantity. Some well-known KGs for Medical Informatics are Open Biomedical Ontologies (OBO) [4], which contains a set of KGs with high level information about medical data which mostly focuses on protocols and treatments, ICD-10 TM Ontology [5], which is a knowledge base created from the Thai modification of the World Health Organization International Classification of Diseases and Related Health Problems. One can have a more complete view over the ontologies for Medical Informatics by reading the survey of Ivanovic and Budimac [6].

Some studies that can be considered closer to our case, are KGs for cancer and specific types of cancer. For instance, the studies [7], [8] propose two ontologies with more or less the same characteristics, those of prognosis of various types of cancer and treatment after the case has occurred. These studies eventhough more general than our case, do not contain information about the various types of skin cancer, and therefore do not serve the same purpose as our study. Next, the following studies, do focus on a specific type of cancer but is different from our case; in [9] the authors model information for liver cancer, in [10] knowledge is represented for breast cancer, and in [11] the authors provide a KG for prostate cancer.

Finally, the COVID-19 KG [12], was also constructed in order to improve the semantic interoperability of the literature about the current pandemic. Nevertheless, our Skin Cancer KG refers to a completely different type of disease.

III. A Knowledge Graph for Skin Cancer Recognition

In this section, we describe in detail the schema of the Skin Cancer KG. In more detail, we analyze each class and object type property at a conceptual level. Next, we present how the data integration mechanism translates data from various datasets into instances of the KG. We also, briefly present the various competency questions on which an information retrieval mechanism can be constructed. Finally, we describe the architecture of the CV model that is used in our use case scenario. The Skin Cancer KG along with any script that was developed for this paper can be found here[2]. In Figure 1, we can see the pipeline of our framework.

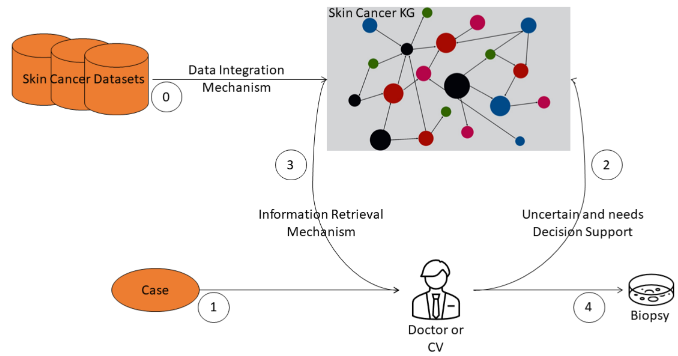

Fig. 1. Framework for the Skin Cancer Knowledge Graph

In Figure 1, we can see that the data integration mechanism maps metadata information into the Skin Cancer KG. Notice that this should be done prior to any use of the information retrieval mechanism, for this reason this is diplayed as step 0. Moreover, if new data needs to be inserted this can be performed at a subsequent moment. After the population of the KG for any case (step 1) that the doctor is uncertain of (s)he can ask from the KG for decision support (step 2), and the information retrieval mechanism will return similar cases (step 3), in order to decide if (s)he should move with a biopsy (step 4). Notice in this paper the doctor is simulate with a CV mechanism.

A. Skin Cancer Knowledge Graph

In this subsection, we give a high-level overview of the KG schema's structure (i.e., the Skin Cancer ontology) and the guiding principles of each class. You can find the KG and the programs created to populate it here[2]. A high-level overview of the main Skin Cancer ontology classes is shown in Figure 2. An instance of the KG can be found here[3].

- **CancerType:** Is the main class which has as subclasses the various skin cancer types.
- **BasalCell:** Is the class that refers to bcc skin cancer cases.
- **SquamousCell:** Is the class that refers to scc skin cancer cases.
- **Melanoma:** Is the class that refers to mel skin cancer cases.
- **Symptom:** This class refers to all the symptoms that are associated with the skin cancer.

[2]https://github.com/dogoulis/kg_visual_skin_cancer
[3]http://lod.csd.auth.gr:7200/

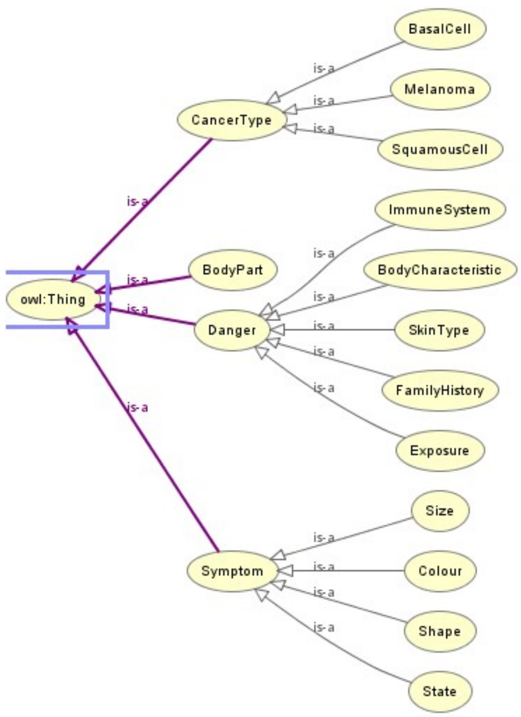

Fig. 2. Skin Cancer Ontology Overview

- **State:** This class, refers to symptoms that have to do with the state of the case, such if it is bleeding, if it painful, if it has a waxy surface, among others.
- **Size:** This class, refers to symptoms that have to do with the size of the case, i.e., its diameter if it changes over time, among others.
- **Colour:** This class, refers to symptoms that have to do with the colour of the case.
- **Shape:** This class, refers to symptoms that have to do with the shape of the case, i.e., if it is asymmetric, if it is a bump, etc.
- **BodyPart:** Indicates where the case is located on the individual.
- **Danger:** This class refers to all the dangers that are associated to provoke skin cancer.
- **ImmuneSystem:** This class, refers to immune system characteristics that are associated to provoke skin cancer.
- **FamilyHistory:** This class, refers to family and personal history characteristics that are associated to provoke skin cancer.
- **SkinType:** This class, refers to skin type characteristics that are associated to provoke skin cancer.
- **BodyCharacteristic:** This class, refers to general body type characteristics that are associated to provoke skin cancer, such as body fat, age, gender, etc.
- **Exposure:** This class, refers to the dangers that the individual was exposed to, which are known to provoke skin cancer.

We also analyze the purpose of the various *object type* properties, i.e., properties that connect instances from one class with instances from another class. Finally, the namespace chosen for this KG is *skin*.

- **hasDanger:** This property relates the cancer types with the dangers that it provokes them. This property has the sub-properties **inBodyCharacteristic**, **inImmuneSystem**, **inSkinType**, **inExposure**, and **inFamilyHistory**, which relate the cancer type, with the body characteristics, the immune system, the skin type, the exposures, and the family history, respectively.
- **isLocated:** This property indicates where the cancer case is located.
- **hasSymptoms:** This property relates the cancer types with the symptoms that they have. This property has the sub-properties **hasSize**, **hasState**, **hasColour**, and **hasShape**, which relate the cancer type, with the size, state, colour, and shape symptoms, respectively.

B. Data Integration Mechanism

The data integration mechanism is a translator of the metadata that exist in a skin cancer dataset to instances of the knowledge graph. In more detail, the data integrator will translate the characteristics of each skin cancer case into Turtle format that can be inserted into the KG.

We will present the intuition of the mechanism through a trivial example. Let us consider a melanoma case ($mel1$) which is of colour black, it is asymmetric, and it has a bump. This information after is processed by our data integration mechanism will be translated in RDF Turtle as follows.

```
skin:mel1 rdf:type skin:Melanoma.
skin:mel1 skin:hasColour skin:colourMel1.
skin:colourMel1 rdf:type skin:Colour.
skin:colourMel1 skin:colour
        "black"^^xsd:string.
skin:mel1 skin:hasShape skin:shapeMel1.
skin:shapeMel1 rdf:type skin:Shape.
skin:shapeMel1 skin:isAssymetric
        "True"^^xsd:boolean.
skin:shapeMel1 skin:hasBump
        "True"^^xsd:boolean.
```

Notice that this is a toy example, and it does not show all the capabilities of the data integration mechanism which can map information for 44 different symptoms, and 27 dangers that may provoke the skin cancers. Nevertheless, we also have to note that there is only a handfull of datasets that contain information about characteristics (i.e., metadata) of the skin cancer cases, as most datasets are oriented for CV problems and therefore contain only images.

C. Information Retrieval Mechanism from Skin Cancer Knowledge Graph

The information retrieval mechanism from the Skin Cancer KG refers to a set of Competency Questions (CQs), gathered by doctors for the most crucial information that they would like from a decision support system to provide. Currently, we have gathered a set of 31 competency questions which can be found here[2], and a smaller set is displayed in Figure 3.

CQ1	What are the symptoms for bcc?
CQ2	What are the dangers to provoke bcc?
CQ3	I have the symptoms A,B,C are these related to scc?
CQ4	I have the body characteristic X with what symptoms of mel is related?
CQ5	I have the family history X with what symptoms of bcc is related?
CQ6	I have the skin type X with what symptoms of bcc is related?
CQ7	I have been exposed to X with what symptoms of scc is related?
CQ8	I have the characteristic of the immune system X with what symptoms of scc is related?
CQ9	What are the symptoms for mel?
CQ10	What are the dangers to provoke scc?

Fig. 3. Set of Competency Questions

Therefore, in order to access the information in the KG for the aforementioned CQs each one of them was translated into a SPARQL counterpart. For instance, the SPARQL counterpart for the CQ6 from Figure 3 can be found in Example 1.

Example 1:

SELECT ?propertySize ?valueSize
?propertyState ?valueState ?propertyShape
?shape WHERE{
?basal rdf:type skin:BasalCell .
?basal skin:hasSymptoms ?symptoms .
?basal skin:hasSize ?size .
?basal skin:hasShape ?shape .
?basal skin:hasColour ?colour .
?basal skin:hasState ?state .
?size ?propertySize ?valueSize .
?state ?propertyState ?valueState .
?colour ?propertyColour ?colour .
?shape ?propertyShape ?shape .
?basal skin:inSkinType ?skinType.
?skinType skin:typeOfSkin ?type
Filter (str(?type) = “Input”) }

D. Computer Vision Mechanism for Skin Cancer Detection

The CV Mechanism that was used in our experiments is *ResNet50* [13]. It is a deep convolutional neural network which has achieved state-of-the-art performance on the ImageNet classification task [14]. Specifically, it is a 50-layer network, consisting of a series of convolutional, batch normalization, and rectified linear unit (ReLU) layers, followed by global average pooling and a fully connected layers as well as residual blocks (which is the core architectural scheme of ResNet models). It is commonly used as a base mechanism for other computer vision tasks, such as object detection and segmentation. One of the key innovations in ResNet50 is the use of skip connections, which allows the network to learn more efficiently and avoid the vanishing gradient problem. In our task, the mechanism was initialized with the pretrained weights of ImageNet, since it generally produces faster and better convergence. Moreover, since we focused on the binary classification task for discriminating between melanoma (mel) and basal cell carcinoma (bcc) types of skin cancer, we replaced the final linear layer with a linear layer that projects the data to the $\mathbb{R}^2$ space. The loss that was used for the optimization of the mechnism is the Binary Cross Entropy loss which is formally defined as:

$$L_{BCE}(y_i, \hat{y}_i) = -(\hat{y}_i * log(y_i) + (1 - \hat{y}_i) * log(1 - y_i)) \quad (1)$$

In terms of optimization, we used the AdamW optimizer [15], and a linear step scheduler for a smoother convergence in the optimal weights. AdamW is a variant of Adam [16] that is designed to improve the performance of the original algorithm, by using a more effective weight decay regularization approach and allowing the weight decay and learning rate hyperparameters to be tuned independently.

IV. Use Case Scenario

In this section we will give a use case scenario, by demonstrating how a doctor can get decision support from the Skin Cancer KG, when (s)he is not sure about a case which may or may not be skin cancer. Based on the returned information from the KG the doctor can get help in order to decide if (s)he finds it rational to proceed with a biopsy or not.

In our case the doctor will be simulated by the CV mechanism that was presented in subsection III-D. Notice that the purpose of our CV mechanism was not to achieve state of the art accuracy scores, such as [17], but rather to simulate more accurately a real life scenario in which a doctor can not have a classification confidence of 99% over all cases.

Given the potential skin cancer case shown in Figure 4, for which the doctor suspects that it is a basal cell carcinoma in a female patient, the symptoms found in Table I were recognized.

Fig. 4. Potential Basal Cell Carcinoma

Then, an information retrieval mechanism which uses our KG, can retrieve images from patients with identical symptoms and gender, or the symptoms can be tuned in order to have more plurality in the answers returned. Lets consider that the doctor wants exactly the same symptoms for the answers returned, then our KG will provide the images shown in

TABLE I
SYMPTOMS FOR POTENTIAL BASAL CELL CARCINOMA OF FIGURE 4

Symptom
has itch
is growing
it hurts
has asymmetric shape
is bleeding
has a bump

Figures 5, 6, and 7. Notice that here we display only the first three results returned by our KG; there is an option to return more.

V. EVALUATION

In this Section we present how we evaluated the completeness and consistency (subsection V-A), and how we evaluated the CV data driven mechanism which was used in Section IV to simulate the doctor which is not sure about a diagnosis (subsection V-B).

A. Completeness and Consistency of the Knowledge Graph

Competency Questions (CQs) compiled during the creation of the official ontology requirements specification document (ORSD) were used to assess the completeness of the Skin Cancer KG [18]. For this reason, we found information from a group of specialists, i.e., doctors, the most important information that is desired from a decision support system for skin cancer to provide. The completeness of the Skin Cancer KG was found adequate, as each CQ when translated into a SPARQL counterpart returned the desired information.

In addition to the CQs, we carried out a validation process to examine the syntactic and structural quality of the KB's metadata and to verify their consistency. Custom SHACL consistency checking rules and native ontology consistency checking. One can find constraint violations, such as cardinality inconsistencies, incomplete, or missing information. Out of 56 SHACL rules, 12 of which referenced to object type properties and 44 to data type properties, the consistency of the Skin Cancer KG was deemed sufficient because none of them returned any rule invalidation. We also looked for instances that belong to the intersection of classes because we did not want that to happen, but none were found. An exemplary shapes constraint is shown below which unfolds a constraint which dictates that all targeted instances of the class "State" will always have at most one boolean value in their datatype property ":isUlcer".

```
skin:ulcerInstance rdf:type sh:NodeShape;
    sh:targetClass skin:State;
    sh:property [
    sh:path skin:isUlcer;
    sh:datatype xsd:boolean;
    sh:maxCount 1;
    ].
```

Fig. 5. First Basal Cell Carcinoma

Fig. 6. Second Basal Cell Carcinoma

Fig. 7. Third Basal Cell Carcinoma

B. Computer Vision Mechanism Evaluation

The mechanism was initially trained on a subset of the HAM10000 dataset, which contained the bcc and mel types of cancer. Bcc, mel and scc types of cancer are the three most common types of skin cancer but the latter one was not contained in the HAM10000 dataset. Hence, we trained and evaluated the mechanism in bcc and mel which is common on both datasets. Following this, the subset was split to 80% for the training dataset and 20% for the validation dataset. The training process lasted for 50 epochs and the weights that resulted to the smaller validation loss were kept as the final mechanism. During training, each image was resized at 256×256 pixels, and a Horizontal Flip with a probability of $p = 0.5$ was performed. Finally, the images were normalized in $[0, 1]$ before being passed to the mechanism. The best validation accuracy resulted in $acc = 95.8\%$. The CV mechanism was tested with some completely new images of skin cancer cases extracted from [3]

Then, the mechanism was evaluated in the second dataset, i.e. in totally unseen images during training. Since the mechanism was trained for mel and bcc types of skin cancer, we also selected the corresponding classes from the second dataset. The evaluation accuracy resulted in $acc = 78.9\%$.

VI. Discussion and Conclusion

In this paper, we presented a KG for the various types of skin cancer, which can represent information about the symptoms and risks of the most common, based on cases, types of skin cancer. Moreover, we provide a data integration mechanism that can map information from various datasets with skin cancer cases into the skin cancer ontology. A use case scenario in which the knowledge graph can be used as a decision support system by doctors, is provided, in which a CV simulates a doctor. The CV mechanism in the cases that is not able to classify the case it can consult the KG to retrieve similar cases based on the characteristics of the one that has at hand.

The Skin Cancer KG was developed in order to assist doctors in general, over their diagnosis of potential skin cancer cases. In other words, the KG is set to help doctors as a decision support system in potential skin cancer cases that they are uncertain if it is a positive or negative case, before moving to a biopsy.

Regarding the evaluation, our goal was, on the one hand, to evaluate the completeness and the consistency of the Skin Cancer KG, and on the other hand the evaluation of the CV data driven mechanism which simulated the doctor. The completeness of the KG (Section V-A) was evaluated with CQs, which were collected by domain experts. More specifically, we translated each CQ into a SPARQL query, and we expected each one to return results, which happened and this shows that our KG can provide crucial information in a disaster management scenario. This is evidence that our KG may deliver significant information to a doctor in order to decide if (s)he needs to move forward with a biopsy. The consistency of the KG (Section V-A) was evaluated with a set of 56 SHACL validation expressions (shapes), and none of them returned any invalidation of the rule. Moreover, we checked if there exist instances which belong to intersection of classes, and there were not any. This shows the consistency of our KG, which indicates that it does not contains noisy and conflicting information. This demonstrates the coherence of our KG, proving that it is free of noise and contradicting information.

In terms of future work, we plan to make the knowledge in the Skin Cancer KG richer by adding information for more skin cancer types, as well as knowledge about their treatment. Next, we also want to extend the information that we can retrieve by defining more CQ and constructing an information retrieval mechanism that will automatically address these queries to the KG. Finally, we will populate the KG with more instances and test it with real doctors in order to show its true value.

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