Interpretable Deep Neural Networks and Bayesian Inference for Orthodontics

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Article

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Abstract: Artificial Intelligence (AI), Machine Learning (ML), and more specifically Deep Neural Network (DNN) have enabled numerous applications in health related science, and more specifically in dentofacial orthopedics, for diagnosis and clinical decision-making support. DNNs and particularly Convolutional Neural Networks (CNNs), powered by the perturbation and saliency maps such as Class Activation Mapping (CAM) and its variants such as Score-CAM have become very popular tools, in medical community thanks to the interpretability of these methods. They are used in particular to locate biomarkers, i.e., observable or measurable signals that reflect the presence, severity or evolution of a disease and that can be considered as discriminating regions in abnormal images.
For orthodontics domain, recent works proposed an innovative methodology coupling DNN and interpretability algorithms to assess cranofacial structures impacted by mandibular retrognathia. Applied to a set of radiographs classified into physiological versus pathological categories, this methodology made it possible to discuss the structures impacted by retrognathia, and to identify new structures of potential interest in medical terms, and to highlight the dynamic evolution of impacted structures according to the level of gravity of mandibular retrognathia.
The main object of this paper is to show how the Interpretable Deep Learning methods combined with Bayesian inference, can be a real "Third Eye" for medical and biological diagnostics in general, and in particular for the orthodontics diagnosis.

Keywords: Orthodontics diagnosis; Cephalometry; Interpretable Deep Learning Neural Network; Artificial Intelligence; Bayesian Inference

1. Introduction

Artificial Intelligence (AI), Machine Learning (ML), Deep Neural Network (DNN) have enabled numerous applications in health related science [1], and more specifically in the focus of this paper, dentofacial orthopedics in the field of diagnosis and clinical decision-making [2]. Indeed, AI has shown to be efficient in identifying cephalometric landmarks, predicting bone age, segmenting teeth, determining the degree of maturation of cervical vertebrae, predicting the need for orthodontic treatment, deciding on extractions or ortho-surgical treatment and assisting in surgical planning [3]. DNNs in general and particularly Convolutional Neural Networks (CNNs) as well as additional interpretable methods of saliency maps such as Class Activation Mapping (CAM) and its variants such as Score-CAM have become very popular tools in medical community thanks to the interpretability of these methods. They are used to locate biomarkers [4], i.e., observable or measurable signals that reflect the presence, severity or evolution of a disease and that can be considered as discriminating

regions in abnormal images [5]. This approach has been applied to various medical fields, such as retinal fundus images, cancer detection, pneumonia detection or Alzheimer's diagnosis. A recurrent and common result of these studies is that DNNs and CNNs outperform practitioners in pathology classification.
Recent works in orthodontics domain [6], proposed an innovative methodology coupling CNNs and interpretability methods to assess craniofacial structures impacted by mandibular retrognathia. Applied to a set of radiographs classified into physiological versus pathological categories, this methodology made it possible:

- to discuss the structures impacted by retrognathia, and already identified in literature, to identify new structures of potential interest in medical terms, and
- to highlight the dynamic evolution of impacted structures according to the level of gravity of mandibular retrognathia (C2Rm).

The main object of this paper is to show how the Interpretable Deep Learning (IDL) methods combined with the Bayesian inference to account for the uncertainties, can be a real "Third Eye" for medical and biological diagnostics in general, and in particular for the orthodontics diagnosis.
The rest of this paper is organized as follows: In Section 2, the main motivation of this work is presented. ...

2. Motivation of the work

Facial skeletal divergence describes vertical disorders of the bone. It refers to the disharmony between the anterior and posterior parts of the facial mass observed in the vertical dimension. One of the notions and subject of research is hyperdivergence and hypodivergence of the bone bases diagnosis.

An architectural difference in the base of the skull according to facial divergence is uncertain and divergent results are found in the literature. The main reasons are several biases which are involved in the cephalometric determination of vertical dysmorphosis such as the precision of the reference points, the intra- and inter-individual variability of the lines and reference points or even the variability of reference standards [7–9].

In addition, the majority of studies conclude on the basis of geometric or topographical correlations carried out between the structure of interest and other skull structures supposed to be impacted by dysmorphosis [10]. But this approach presents methodological limitations and does not allow a global and dynamic representation of all the structures impacted by the pathological process [11].

In this context, it appears relevant to develop new morphometric tools which do not involve defining areas of interest a priori, nor defining shapes using a set of benchmarks, and which allow to follow the dynamic evolution of structures impacted by the severity of a pathological process. It is admitted that structural differences exist at the level of the lower level of the face between the hypodivergent and the hyperdivergent at the level of the posterior and anterior face (REF). See Figure 1.

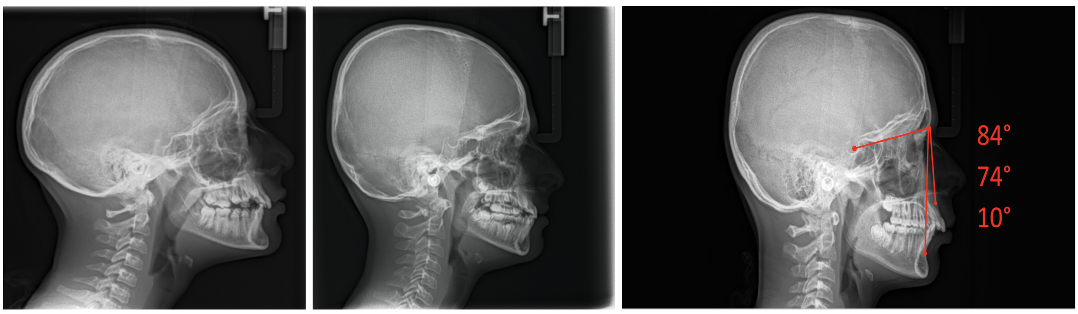

Figure 1. Two cases of facial skeletal divergence and cephalometric angles measurement.

An architectural difference in the base of the skull according to facial divergence is uncertain and divergent results are found in the literature. According to Droel and Isaacson [12], these are more modifications of the glenoid cavity or the head of the condyle than anatomical modifications of the base of the skull. According to Xiao et al. [13] there are no significant differences above the palatal plane between the hypodivergent and the hyperdivergent. According to Rawat et al. [14], Awad et al. [18], by Brondeau [15] and Kasai et al. [16], the angle of flexion of the base of the skull does not play a significant role in the development of vertical skeletal dysmorphoses. According to de Brondeau [24], Ikoma and Arai [17], Kasai et al. [16] and Awad et al. [18], the anterior part of the base of the skull has a major significant impact on the vertical relationships of the face due to its orientation and its length. According to Rawat et al. [14], the posterior part of the skull base is the only basic-cranial parameter to have an impact on the vertical dimension, whereas for other authors (Kasai et al. [16], de Brondeau [15]) the posterior part does not play a role in establishing the vertical facial pattern. Finally, the hyoid bone is closer to the cervical spine in hyperdivergent people, with a reduced distance from the chin. It is also more inclined relative to the SN line and the opposite is observed in the hypodivergent [19]. If the results often appear divergent, it should be noted that several biases are involved in the cephalometric determination of vertical dysmorphosis such as the precision of the reference points, the intra- and inter-individual variability of the lines and reference points or even the variability of reference standards. In addition, the majority of studies conclude on the basis of geometric or topographical correlations [20–22] carried out between the structure of interest and other skull structures supposed to be impacted by dysmorphosis. But this approach presents a certain number of methodological limitations [10,20] and does not allow a global and dynamic representation of all the structures impacted by the pathological process. In this context, it appears relevant to develop new morphometric tools which do not involve defining areas of interest a priori, nor defining shapes using a set of benchmarks, and which allow the dynamic evolution of structures impacted by the severity of a pathological process.

In recent years, the digital revolution and in particular Artificial Intelligence (AI) have enabled numerous applications in dentofacial orthopedics in the field of diagnosis and clinical decision-making support. Indeed, AI is efficient in identifying cephalometric landmarks [23], predicting bone age [24], segmenting teeth [25], determining the degree of maturation of cervical vertebrae [26], predicting the need for orthodontic treatment, deciding on extractions [27] or ortho-surgical treatment [28] and assisting in surgical planning [29].

In many medical imaging, Deep Neural Networks (DNNs) and particularly CNNs powered by the additional interpretable methods of saliency maps such as Class activation mapping (CAM) and its variant Score-CAM have become very popular tools in supervized classification of images. They are used in particular to locate biomarkers, i.e., observable or measurable signals that reflect the presence, severity or evolution of a disease and that can be considered as discriminating regions in abnormal images.

More recently, an innovative methodology coupling CNNs and interpretability algorithms to assess craniofacial structures impacted by mandibular retrognathia (C2Rm) has been published [6]. Applied to a set of radiographs classified into physiological vs pathological categories, this methodology made it possible to : discuss the structures impacted by retrognathia and already identified in literature; identify new structures of potential interest in medical terms; highlight the dynamic evolution of impacted structures according to the level of gravity of C2Rm.

3. General methodology

In this research:

- The first objective is the development of a neural network more efficient than using a single cephalometric angle to define the vertical typology of a patient.
- The second objective is the use of the interpretability of neural networks to answer the following questions:

  1- Do morphological differences exist between a hypodivergent, mesodivergent and hyperdivergent beyond the lower level of the face?

2- If so, what structural factors are likely to be determining in the establishment of a patient's vertical facial pattern?

To achieve these objectives, the following steps are considered:

- Appropriately selecting and labeling the images by an expert using cephalometric angles;
- Design and use an appropriate CNN network to do supervised classification;
- Analyze the classification results with classical measures, and in particular the confusion matrix;
- Analyse the results using CAM techniques and its various variants visualizing well-classified and poorly-classified images (4 cases) for each patient and for all patients in each class (this requires registration of these images). This analysis allows us to see the importance of the anatomical areas which play an important role in the classification.
- By generating the saliency maps using the perturbation method for each case in each class, and computing the mean and the variance maps, we can visualize the mean maps as well as its associated uncertity quantified by the map of variances. These images become biomarkers for presence of the hypodivergent, mesodivergent and hyperdivergent anomalies.
- By analyzing the means and the variances images of the ensemble of cases, we can see if other angles or other cephalometric parameters interpret these good or bad classifications.
- It is only after these steps that we can conclude whether there is a need to redo the entire analysis, starting by redoing the labeling via two angles.
- Another complimentary approach is to do unsupervised (clustering) or semi-supervised classification, and see if the results can correspond to those of supervised methods. Then compare with a labeling using two cephalometric angles.

3.1. Constitution of the learning data base

We collected 23,479 profile radiographs from four French orthodontic clinics between January 2012 and December 2021. This database concerns patients who consulted for dentofacial orthopedic treatment with an aesthetic and/or functional reason, and not presenting congenital or hereditary diseases. The population is made up of 1/3 men and 2/3 women. The average age is (12 +/- 5) years. The lateral radiographs were obtained using a CARESTREAM CS 9000-C X-ray imaging system. The collection and storage of data was carried out in compliance with the GDPR rules and recommendations in force within the European Union. Then, we followed different selections:

First selection: In order to increase the quality and reproducibility of the study, we kept only the lateral teleradiographs respecting the following criteria: skull in standard position included in a cephalostat with the Frankfurt plane parallel to the ground (Silva 2003) ; entire skull with visualization of the cervical vertebrae; patient in occlusion; no splitting of the mandibular edge, excluding positioning errors or asymmetrical patients.11 193 lateral teleradiographs were then retained.

Second selection: To minimize confusion bias, we chose to only include subjects in skeletal class I, based on the measurement of the angle ANB = 2° +/-2° and the AoBo = 2 +/- 2 mm. The weight of the data overwhelms sampling biases linked to gender, ethnicity or age. 2,771 lateral teleradiographs were selected.

Labeling phase: The first step consisted of teaching a convolutional neural network to discriminate between a hypodivergent, mesodivergent and hyperdivergent subject. This learning took place following the presentation of a large number of examples labeled according to their level of divergence. The labeling was carried out by a dentofacial orthopedist practitioners using software allowing the measurement of the GoGn/SN angle (see table 1). This resulted in a base of 2,771 rigorously selected profile teleradiographs allowing training of the network, composed of: 867 hypodivergents, 1408 mesodivergents, 496 hyperdivergents. Figure 2 shows these different steps.

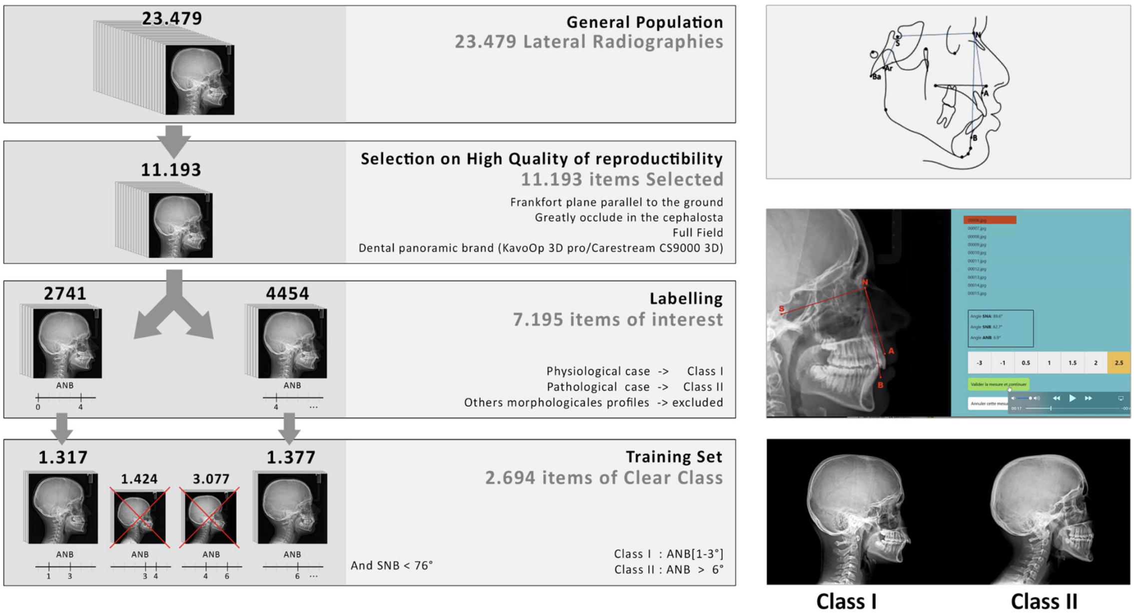

Figure 2. Constitution of the learning data base

3.2. Interpretable Deep CNN Architecture

A first DNN model was designed and trained using 80% of the data and 20% of the data served as a "test" to check the performance of the neural network.

Several standard CNN architectures have been created, comprising between 7 and 9 layers of neurons. In order to increase the classification accuracy, two neural network sub-models were created to differentiate: on the one hand hyperdivergence from mesdivergence (network named "Hyper Network"; and hypodivergence from mesdivergence of another network, named "Réseau Hypo". These networks were exposed to different databases but operated on the basis of the same general principles. This method proved to be unsatisfactory since the performance of the networks created, peaking at 60% (a performance of 50% means that the classification of the image is random).

We then used another method called "transfer learning". Indeed, traditional learning techniques require high computing times and significant resources. On the other hand, "transfer learning" makes it possible to use pre-trained models as a starting point in order to achieve the rapid development of a high-performance neural network for solving problems, particularly in computer vision [122].

In order to detect areas correlated with facial divergence, it is necessary to identify the areas of interest used by the neural network when making decisions. We then chose to use Score CAM [124] as a method of interpretability of the neural network. The latter makes it possible to generate saliency maps highlighting the areas of the image specific to vertical dysmorphosis and therefore used by the neural network to carry out its classification. It combines the use of the CAM (class activation mapping) method and the perturbation method.

The CAM method consists of pooling the different salient elements of the network which contributed to the classification and which are located on the last layers; The last layer shows the globular areas representing the centers of gravity of the areas of importance which can be visualized via a color thermal map corresponding to the importance of the area of the skull for classification. A red zone will be very specific to the dysmorphosis. The blue/green areas are not useful for classification and therefore do not represent elements correlated with the pathology. The methodology used allowed us to achieve a performance of the Hyper and Hypo networks of around 90%. See Figure 3.

The perturbation method consists of altering the image by generating masks on certain areas of the image. It is then a matter of hiding from the network the information which the zone carries. The extent of the impact of this masking on decision-making is representative of the importance of the area. Therefore, the salient features are identified by the CAM method. Then each identified characteristic is used as a mask to identify its importance. The method makes it possible to map areas of importance on the input image with very fine spatial resolution.

We can give a Bayesian interpretation for this process: As we do the perturbations following some prior knowledge, and for each realization, we obtain a map, and this for all the individuals of the same class, we can compute the mean and the variance images. The mean image is used for the main visualization, and the map of the variances show the uncertainties. These informations can be used to make better decisions. However, showing both maps of the means and the variances makes the presentation for the practitioner more difficult to understand.

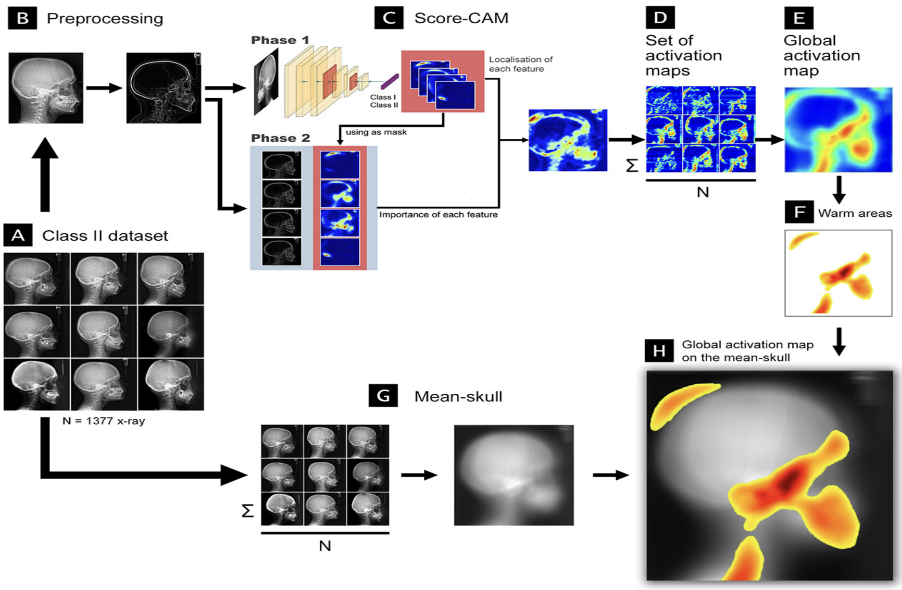

Figure 3. General methodology: Classification, ScoreCAM, Mean over all the images in the same class

4. Main results

The performance of the Hyper and Hypo networks is around 90%. This means that the GoGn-SN angle in itself is not sufficient to diagnose vertical dysmorphosis: 90% of the subjects in the study present consistency between the GoGn-SN angle and the cranio-facial signs of their typology. vertical and 10% of the study subjects present an inconsistency between the GoGn-SN angle and the craniofacial signs of their vertical typology. These 10% correspond to false positives or false negatives from the GoGn-SN angle, and may be due to cephalometric biases, as seen previously and/or operator errors during labeling.

Skeletal divergence is assessed by the values of the three angles GoGn/SN, ENA-ENP/SN and FMA. "Borderline" cases can be diagnosed as hyperdivergent from one angle and mesdivergent from another. For example, faced with a subject presenting an ENA-ENP/GoGn angle of 26° and a GoGn/SN of 34° it will be difficult to classify the subject in the hyperdivergent group. See Figure 4.

A patient qualified as hyperdivergent by angular analysis and mesodivergent according to craniofacial signs. This patient is a false positive, he is diagnosed as hyperdivergent by the GoGn-SN angle (37.2°) while the neural network, based on all the cranio-facial signs, qualifies him as mesodivergent. See Figure 5.

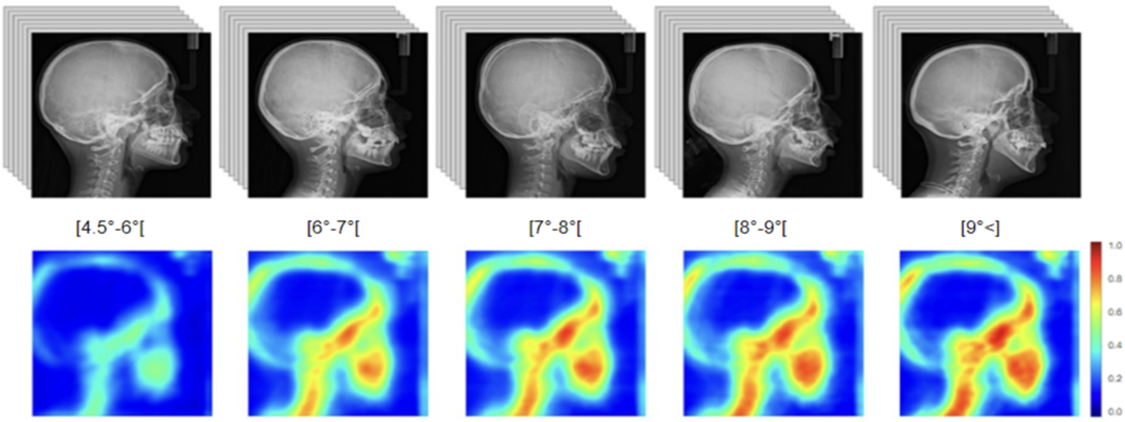

Figure 4. ScoreCAM maps for different classes (different angles).

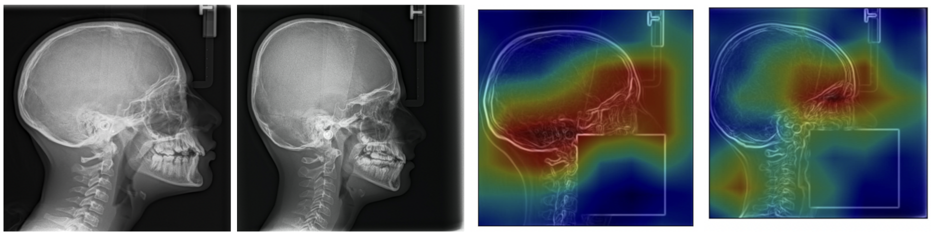

Figure 5. Main result: Two cases and their corresponding scoreCAMs

This tool could be particularly useful for practitioners in determining “borderline cases” during orthodontic assessments of young children in order to offer the best possible therapy and to anticipate abnormal vertical growth, before the installation and worsening of this last.

The areas having contributed most strongly to decision-making (dark red) are as follows: cribriform plate of the ethmoid; crista galli process of the ethmoid The areas having strongly contributed to decision-making (red) are as follows: anterior territory of the base of the skull with the orbitonasal area of the frontal; upper endocranial part of the lesser wings of the sphenoid bone and sphenoid jugum; tubercle of the sella turcica. The areas having moderately contributed to decision-making (orange) are as follows: frontal sinus; Turkic saddle; clean nasal bone; lower vertical part of the frontal bone; posterior curvature of the neck.

The areas that did not contribute to decision-making (yellow, green, blue) are as follows: posterior part of the base of the skull; temporal bone; occipital bone; upper part of the maxilla; cervical spine; cranial vault. The determining structural zones correlated with facial hypodivergence are concentrated in the anterior basal-cranial zone, and in particular at the level of the ethmoidal territory.

The learning curves reveal a success of 90%, meaning that 10% of subjects present a discrepancy between their vertical diagnosis based on the GoGn-SN angle and their craniofacial signs. The GoGn-SN angle is insufficient in the diagnosis of a pathology of the vertical dimension.

When the lower level of the face is masked, the performance of the neural networks approaches 90%, showing that structural signs of vertical dysmorphosis exist beyond the maxillo-mandibular level. The latter concern the entire base of the skull, the petrous pyramids and the upper cervical spine in the hyperdivergent and the anterior basic-cranial part, particularly in its ethmoidal portion in the hypodivergent. See Figure 6.

5. Conclusions

We used the DNN as a "Third Eye" to understand the maps of the area of the head which participate more to the disharmony between the anterior and posterior parts of the facial mass, called hyperdivergence and hypodivergence of the bone bases diagnosis. Starting by labeling the

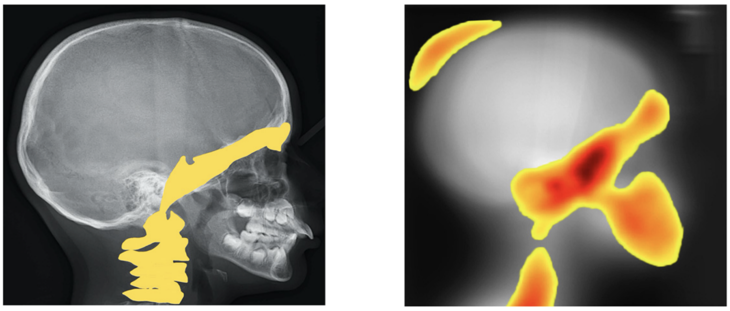

Figure 6. Main result: Correspondance between the structured map correlated with the SNB angle and the Saliency map.

radiographies using one angle on a cephalographic geometry, we used the DNN and the interpretability tools of the classification CNN as a "Third Eye" to visualize the map of the regions of the head which participate more to that classification. This combination of using NNs, ML tools, and the biological prior knowledge, made our method as an AI system for hyperdivergence and hypodivergence of the bone bases diagnosis.

More specifically, the following points have been clarified:

- A clear and synthetic summary of the areas impacted by hypo and hyperdivergence identified in the literature, is presented;
- A global AI method is used to discuss and to give a conclusion to the questions raised by this synthesis.

The main conclusions are:

- There is no consensus on the areas impacted by hypo and hyper divergence (hence the need for our AI approach).
- The GoGn-SN angle is insufficient for a diagnosis.
- The structural signs of vertical dysmorphosis exist beyond the maxillo-mandibular level.

During this study, we could highlight the following points:

- To identify impacted areas more effectively than traditional methods;
- To show the limits of the GoGn-SN angle;
- To show, via the hiding and perturbation technique, that the structural signs of vertical dysmorphosis exist beyond the maxillo-mandibular level.

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