Keywords: polycystic ovary syndrome, PCOS, ultrasound imaging, Neural Networks, grad-CAM, Python programming

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AUTOMATION OF POLYCYSTIC OVARY SYNDROME DIAGNOSTICS THROUGH MACHINE LEARNING ALGORITHMS IN ULTRASOUND IMAGING

Abstract

This article presents a study aimed at using machine learning to automate the analysis of ultrasound images in the diagnosis of polycystic ovary syndrome (PCOS). Today, various laboratory and instrumental methods are used to diagnose PCOS, including the analysis of ultrasound images performed by medical professionals. The peculiarity of such analysis is that it requires high qualification of medical professionals and can be subjective. The aim of this work is to develop a software module based on convolutional neural networks (CNN), which will improve the accuracy and objectivity of diagnosing polycystic disease as one of the clinical manifestations of PCOS. By using CNNs, which have proven to be effective in image processing and classification, it becomes possible to automate the analysis process and reduce the influence of the human factor on the diagnosis result. The article describes a machine learning model based on CNN architecture, which was proposed by the authors for analyzing ultrasound images in order to determine polycystic disease. In addition, the article emphasizes the importance of the interpretability of the CNN model. For this purpose, the Gradient-weighted Class Activation Mapping (Grad-CAM) visualization method was used, which allows to identify the image areas that most affect the model’s decision and provides clear explanations for each individual prediction.

1. INTRODUCTION

Polycystic ovary syndrome is one of the most common endocrine pathologies affecting women of reproductive age worldwide. Characterized by hormonal imbalance and the
presence of cysts in the ovaries, this disease causes a variety of complications and health problems (Bulsara et al., 2021). The prevalence of PCOS is striking, as it affects approximately 5-15% of women of reproductive age (Azziz, 2016; Liu et al., 2021). Moreover, the range of 5-15% is a kind of averaged range, since different studies give different values. World Health Organization data indicate that 70% of PCOS cases worldwide remain undiagnosed (World Health Organization, 2023). Despite numerous studies, the exact causes of PCOS are still unknown, but there is a hypothesis that genetic and environmental factors interact (Hoeger et al., 2021).

The impact of PCOS on women's fertility has important social and demographic implications. Women suffering from this syndrome often face problems with natural conception, and many of them need to resort to the use of assisted reproductive technologies, such as in vitro fertilization. In addition, PCOS is associated with the risk of developing long-term diseases such as type 2 diabetes and cardiovascular disease, which can negatively affect the quality and duration of life. Early diagnosis of PCOS plays an important role in further treatment and elimination of the disease's consequences (Garad & Teede, 2020).

PCOS is associated with a disorder of folliculogenesis (Rasquin et al., 2022). PCOS has a multifactorial nature and is characterized by a several clinical manifestations, including not only polycystic disease, but also hyperandrogenism, oligo-ovulation or anovulation, and others. Since PCOS is a multifactorial disease with various manifestations, there is no single diagnostic criterion for defining this disease (Sirmans & Pate, 2013; Christ & Cedars, 2023).

In the context of these challenges, accurate and timely diagnosis of PCOS is particular importance. Transvaginal ultrasound is the leading method for visualizing and analyzing the pelvic organs, particularly the structure of the ovaries. Some of the criteria that indicate PCOS during analyzing ultrasound images are listed below:

- Number of follicles: according to the Rotterdam diagnostic criteria (Rotterdam ESHRE/ASRM, 2004), the presence of more than 12, and according to other recommendations (Teede et al., 2018), more than 20 small follicles (2-9 mm in diameter) in each ovary;
- Ovarian volume: an increase in ovarian volume (more than 10 cm3) may also indicate polycystic disease (Rotterdam ESHRE/ASRM, 2004);
- Echogenicity of the ovarian stroma: in the case of PCOS, the stromal area of the ovary on ultrasound images is often displayed as a hyperechoic (Dwivedi et al., 2019) and denser area, which may be associated with increased androgen production.

Regarding the above criteria, it should be noted that each of them alone does not indicate PCOS. They should be considered in combination (Gyliene et al., 2022). For example, polycystic ovaries can also occur in healthy women who are not diagnosed with PCOS.

It is obvious that high-quality analysis of ovarian ultrasound images is the key to accurate diagnosis of polycystic disease as one of the important markers of PCOS. However, it is also obvious that this analysis often depends on the subjective interpretation of specialists. Thus, there is an urgent task to develop an artificial intelligence system that would automate the process of analyzing ultrasound images and reduce the influence of the subjective factor on the result, which will open new horizons for improving the accuracy of PCOS diagnosis.

The main goal of this research is to create a robust deep learning model that can analyze ultrasound images and accurately classify the presence or absence of polycystic disease.

However, in addition to the classification itself, the authors also aim to implement functionality that will allow to highlight key areas in the image on which the deep learning
model made its prediction. This will not only simplify the interpretation of the analysis results for medical professionals, but also provide additional insight into the logic of the model. To implement this functionality, the Grad-CAM method is used, which is an important tool for visualizing the impact of certain areas of the image on the final decision of the neural network (Selvaraju et al., 2020). With Grad-CAM performs pseudo-segmentation of the original images, which allows not only to increase the efficiency of the diagnostic process but also to ensure its transparency and objectivity.

2. METHODOLOGY

2.1. Data description

The collection and processing of primary medical images is a complex process (Esteva et al., 2021), due to the need to digitize medical images, adhere to confidentiality, ethical standards, and in some cases the need to obtain patient consent for the use of their data. The problem of finding datasets is especially acute in the context of developing a deep learning model, training it, and validating the results. Datasets may not exist, they may be incomplete or contain too few elements, they may be closed or require paid access, etc. In the context of solving the problem of diagnosing polycystic disease, the authors analyzed various databases on the Internet and found an open dataset "PCOS detection using ultrasound images" on the Kaggle platform (Choudhari & Korde, 2022). This dataset was used in further research. However, it is worth noting that Kaggle does not provide detailed information about the origin of this data, which may limit the depth of the analysis and conclusions.

Table 1 provides information that shows the structure and size of the "PCOS detection using ultrasound images" dataset, as well as the distribution between the various categories and classes included in the analysis. This table is key to understanding the balance and representation of different categories in the data that are analyzed.

<table>
<thead>
<tr>
<th>Tab. 1. Structure and size of the dataset</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training set</td>
</tr>
<tr>
<td>781</td>
</tr>
<tr>
<td>Test set</td>
</tr>
<tr>
<td>Total</td>
</tr>
</tbody>
</table>

2.2. Data augmentation

The dataset available for our analysis contains a total of 3846 ultrasound images, of which 1924 belong to the training set and 1922 - to the test set (in fact, there are 10 more images in the dataset, but these 10 images are damaged and cannot be used for analysis). This amount of data may not be enough for effective training and implementation of the neural network model. Therefore, in order to increase the sample size, augmentation was applied to the original dataset, which plays a key role in improving the accuracy and reliability of the machine learning model, especially in cases where the amount of primary data is insufficient.

Augmentation involves creating modified versions of existing images using various transformation techniques. These transformations can include such changes as rotation, shift,
scaling, contrast modification, mirroring, and other similar operations. The result is new images that remain relevant to the training, but at the same time add additional diversity to the training set.

This approach allows to expand the training set, increasing its diversity and improving the model's ability to generalize. This is important because a model trained on more diverse data is better able to adapt to new, previously unknown cases encountered in real-world applications. The use of data augmentation may provide a more robust and accurate model for classifying ultrasound images for the diagnosis of polycystic disease.

The augmentation and preprocessing were performed according to the rules shown in Table 2. It is important to note that the additional data obtained through augmentation is added to the image set during training and validation, forming the appropriate batch size in each epoch.

Tab. 2. Augmentation and preprocessing rules

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normalization</td>
<td>Division by maximum</td>
</tr>
<tr>
<td>Shift range</td>
<td>±40%</td>
</tr>
<tr>
<td>Zoom range</td>
<td>±40%</td>
</tr>
<tr>
<td>Horizontal mirroring</td>
<td>Allowed</td>
</tr>
<tr>
<td>Vertical mirroring</td>
<td>Allowed</td>
</tr>
<tr>
<td>Rotation range</td>
<td>60° from the vertical axis</td>
</tr>
<tr>
<td>Training set</td>
<td>60%</td>
</tr>
<tr>
<td>Validation set</td>
<td>40%</td>
</tr>
<tr>
<td>Filling method</td>
<td>Fill with nearest</td>
</tr>
</tbody>
</table>

2.3. Description of the developed neural network model

In this project, the CNN architecture was used, which has proven to be very successful in image-based classification tasks (Chai et al., 2021), including medical images (Kshatri & Singh, 2023; Yamashita et al., 2018). To create a neural network model and visualize its operation, the authors used the Python programming language and the following libraries: TensorFlow, Scikit-learn, NumPy, pandas, matplotlib, OpenCV.

Initially, the authors tried to use pre-trained networks with the ResNet architecture (ResNet50/101/152), but these models did not perform satisfactorily due to overtraining or low accuracy on the samples. They also considered using the autogluon framework for automated model training, but abandoned this idea due to limitations in the use of Grad-CAM and other visualization methods.

Therefore, the authors developed their own machine learning model based on the CNN architecture. The structure of this model is shown in Table 3.
The developed model takes as input an image of 224x224 pixels in three RGB color channels. During processing, the image goes through three consecutive two-dimensional convolution operations, each of which is accompanied by a 4x4 pooling operation to reduce the dimensionality by the maximum value. All convolutions use the ReLU (Rectified Linear Unit) activation function, which is described as:

\[ f(x) = \max(0, x) \]  

where: \( x \) - input value.

The ReLU activation function is used to introduce nonlinearity into the model, returning 0 for all negative values and the input value for positive values.

After this step, the features are convolved back into a vector of 72 elements and passed through two fully connected layers. The first layer uses ReLU activation, while the final layer has a sigmoid activation function defined as:

\[ f(x) = \frac{1}{(1+\exp(-x))} \]  

Sigmoid function transforms values into a range between 0 and 1, making it ideal for binary classification tasks (Hassaballah & Awad, 2020).

It is important to note that the total number of training parameters in the developed model is 9452 (see Table 3), which is significantly less compared to complex architectures such as ResNet or VGG16/19. This simplicity of the model reduces the risk of overtraining, especially in the last stages of training, making it more stable when used with new data. The structure and set of layers of the neural network model are justified by the fact that cysts have a large area on ultrasound images, so we can build large enough sections during convolution.

3. RESULTS

3.1. Training and validation accuracy

To train the developed machine learning model described in the previous section, the training dataset with ultrasound images of the ovaries was divided into training and
validation sets in the proportion of 60% and 40%, respectively (thus, 1155 images with and without polycystic disease were randomly assigned to the training set, and 769 - to the validation set).

Fig. 1 shows the plots of the loss function (binary cross-entropy) and model accuracy on the training and validation sets at each epoch.

As can be seen from the above graphs, the model achieved high accuracy in accordance with the validation data after the fourth epoch, which indicates the absence of both overtraining and undertraining. At the tenth epoch, the accuracy of the model on the training set was 0.9905, while on the validation set it was 0.9909, which indicates a high overall efficiency of the model.

In the next step, the trained model was applied to the test set. As a result, a confusion matrix was obtained (Table 4), where the cells reflect the correlation between the actual classes and the model predictions. The accuracy of the model calculated from this data is 99.7%.

Tab. 4. Confusion matrix

<table>
<thead>
<tr>
<th></th>
<th>Polycystic ovary</th>
<th>Normal ovary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polycystic ovary</td>
<td>777</td>
<td>1</td>
</tr>
<tr>
<td>Normal ovary</td>
<td>4</td>
<td>1140</td>
</tr>
</tbody>
</table>

3.2. Visualization of model predictions

The Grad-CAM method allows to understand which areas in the input image are crucial for the model's prediction by highlighting them with a heat map. The visualization process using Grad-CAM goes through several stages:

1. First, the CNN is trained to distinguish between different classes of images (in our case, between images with and without polycystic disease).
2. During the analysis of a particular image, the model calculates gradients relative to the predicted class, which allows us to determine which factors have the greatest impact on the decision.

3. These gradients are used to weight the feature maps obtained in the last convolution layer to determine the contribution of each feature to the final prediction.

4. Subsequently, the aggregation of these weighted feature maps is displayed in the form of a heat map, where areas with higher values show the key areas that influenced the model's decision.

Figure 2 shows the result of applying the Grad-CAM method to the ultrasound images belonging to the testing set. To improve the displaying of information, in the study used interpolation of the activation map and its overlay on the original image in the form of contours.

![Example of ultrasound images with contours highlighting the areas that most influenced the model's decision to detect polycystic disease: left - source image, center - activation map, right - output image](image)

With Grad-CAM, it is possible not only to check the validity of the neural network model, but also to understand the logic behind its decisions by visualizing those areas in the image that are considered the most informative for determining the presence of polycystic disease. This provides a valuable tool for interpreting decisions, making the model not only effective but also understandable for medical professionals.
4. DISCUSSION

Despite the high accuracy of the developed model, as well as the clarity of interpretation of its solutions, some certain aspects and challenges deserve further discussion. The authors encountered problems related to the limitations of available data and the need for data augmentation, which affects the overall ability of the model to generalize new data. Moreover, a detailed visual analysis of the used dataset showed that it initially contained hundreds of variations of several base images (this may indicate that the dataset was already augmented). Therefore, a very high model accuracy of 99.7% was achieved on the test data, as it is quite homogeneous. Overall, based on the results of the presented work, the authors would not recommend using the "PCOS detection using ultrasound images" dataset for further use and design of new and more powerful machine learning models, as the dataset is not representative.

Another challenge is the choice of neural network architecture and its settings, which directly affect the efficiency and accuracy of the model. Obviously, given the shortcomings of the dataset used, the developed machine learning model will have to be adjusted in the future on a more extensive set.

In this work, only accuracy of the developed model was calculated based on the confusion matrix. However, in future studies, provided that a high-quality dataset is formed and a model is trained on it, it is necessary to analyze other characteristics of binary classification, such as: receiver operating characteristic (ROC) curve (Karpiński et al., 2022), Matthew's correlation coefficient (Chicco et al., 2021; Chicco & Jurman, 2023).

It is also important to emphasize that although the developed model accurately detects polycystic disease on ultrasound images, this ability is not equivalent to the model's ability to diagnose PCOS, as this diagnosis depends on many criteria (Deswal et al., 2020) (see Table 5).

Tab. 5. Criteria to consider when making a PCOS diagnosis

<table>
<thead>
<tr>
<th>Criterion</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polycystic ovary</td>
<td>The presence of twelve or more follicles in one ovary or increased ovarian volume (more than ten cubic centimeters).</td>
</tr>
<tr>
<td>Hyperandrogenism</td>
<td>Elevated levels of androgens in the blood, which can manifest itself through hirsutism, acne, or baldness.</td>
</tr>
<tr>
<td>Oligo-ovulation or anovulation</td>
<td>Irregular ovulation or lack of ovulation, leading to irregular menstrual cycles.</td>
</tr>
<tr>
<td>Insulin resistance</td>
<td>Impaired ability of cells to respond to insulin, often associated with polycystic ovary syndrome.</td>
</tr>
<tr>
<td>Hormonal imbalance</td>
<td>Abnormal ratio of hormones, in particular, increased production of luteinizing hormone compared to follicle-stimulating hormone.</td>
</tr>
<tr>
<td>Ovarian morphology</td>
<td>Changes in the structure of the ovaries that are visible on an ultrasound image, such as an increase in their size.</td>
</tr>
<tr>
<td>Absence of other endocrine disorders</td>
<td>Exclusion of other conditions that may cause similar symptoms, such as excessive production of cortisol or thyroid hormones.</td>
</tr>
</tbody>
</table>

For example, the Rotterdam diagnostic criteria require at least two of the three criteria to be met for the diagnosis of PCOS: polycystic ovaries, hyperandrogenism, and oligo- or
anovulation (Rotterdam ESHRE/ASRM, 2004). The developed neural network model is able to effectively identify only one of these criteria, polycystic ovaries, based on the analysis of ultrasound images.

For a complete diagnosis of PCOS, it is also necessary to assess the level of relevant hormones and physiological signs, which the model cannot determine due to its limitations on image analysis alone. Thus, although the developed model is a valuable tool for preliminary screening and detection of potential polycystic ovary disease, it cannot independently diagnose PCOS. This emphasizes the importance of a comprehensive approach to diagnosis that includes both clinical examination and laboratory tests, as well as instrumental assessment methods, allowing medical professionals to obtain a complete picture of the patient's condition.

Analyzing the effectiveness and reliability of the developed neural network model in the context of PCOS diagnosis, it is worth noting that the model demonstrated high accuracy in classifying ultrasound images. In particular, we observed that the model is not prone to overtraining or undertraining, which is a positive aspect, guaranteeing its stable performance on the data set that was available to us.

However, it is necessary to take into account the limitations of the data set used. The presented analysis is based on a relatively homogeneous dataset that does not capture the wide range of possible ultrasound image variations associated with PCOS. This poses a risk that the model may not demonstrate the same high accuracy and reliability when applied to more diverse data that include a wider range of syndrome variations.

Accordingly, to further develop and improve the study, it is critical to expand the data sample. This means including more ultrasound images representing different forms and stages of PCOS, as well as images of patients with different physiological characteristics. The variety of images will allow the model to better generalize and adapt to new data, increasing its efficiency and reliability in a wide range of clinical scenarios.

Thus, despite the high accuracy of the model on a limited sample, it is important to remember the necessity of expanding and diversifying the data to further improve the quality of PCOS diagnosis. This will help improve the model and make it not only accurate but also universal, i.e., able to work effectively with a variety of clinical cases.

5. CONCLUSIONS

The paper describes in detail the processes of data preparation, model training, and visualization using Grad-CAM, which allowed not only to determine the presence of polycystic disease but also to understand the basis on which the model makes its predictions.

Although experiments have shown that the developed neural network model demonstrates an accuracy of 99.7% when detecting polycystic disease, it is important to note that its effectiveness is limited by the data set on which it was trained. Therefore, in this study, the authors do not focus on the achieved accuracy, but rather aim to show the benefit of using the Grad-CAM technique, which allows visualizing the image areas that influence the model's decisions, ensuring the interpretability of its predictions. This study emphasizes how advanced technology can contribute to the early detection of polycystic disease, although additional clinical data must be considered for a complete diagnosis of PCOS.
Further research can be carried out in several directions. First, it is imperative to increase and diversify the data sample for model training and validation to improve their ability to generalize and adapt to new data. Secondly, it is necessary to add the ability to automatically count the number of follicles in the ultrasound image and calculate the ovarian volume. Thirdly, the development of hybrid models that integrate machine learning with clinical parameters can contribute to the creation of more comprehensive innovative PCOS diagnostic systems based on artificial intelligence. Fourth, the interpretability of machine learning models needs to be further investigated and methods for explaining model predictions need to be developed to facilitate better acceptance of these technologies in the medical community.

REFERENCES


