Characterization of Sprays by Image Recognition with Neural Networks

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Abstract
For quality control of medical spray nozzles, control systems must be capable of characterizing sprays based on droplet size distribution. Image analysis methods are a powerful tool for characterizing a spray very quickly and with a high degree of confidence. This work aims to develop a sensor system for the characterization of sprays via Convolutional Neural Networks (CNN), a subcategory of machine learning. Images of sprays conducted by a CCD camera, and the drop size distribution measured via laser diffraction. Subsequently, CNNs have been successfully trained to assign each image to one five spray categories, each represented by a mean droplet diameter ($d_{50,3}$) and with a range variation of 20 µm. Furthermore, drop size distributions have been assigned by analyzing spray images via CNNs with a deviation of each class of 0.1 – 1.5 % compared to the measured value.

Keywords
Nasal spray, drop size distribution, Convolutional Neural Network, quality control

Introduction
Medical spray pumps for pharmaceutical application are widely used as an alternate route of administration for systemic therapy in place of intravenous routes. Singe phase swirl nozzles (hollow cone ore full cone nozzles) are used in medical pumps and their drop size distribution, as well as the spray plume geometry, strongly depends on the nozzle geometry.
Spray parameters are commonly the design target of medical spraying systems or must be controlled in the process. To control the spray parameters, reliable and preferably non-invasive sensor systems are needed. Regarding the high production numbers of application apparatuses for nasal sprays, it is obvious that these sensor systems should provide highly time-resolved data to ensure quality by in-line measurements.
Neural networks (NN) are a subcategory of machine learning. NNs consist of a stack of layers, each one having various numbers of neurons or nodes connected with the nodes in the previous and following layer, forming a so-called dense layer. These connections are weighted, and structural changes can be accomplished by adjusting those weights (Fig.1).
Convolutional neuronal networks (CNNs), were successfully applied in fields like face detection, autonomous driving [1], and cancer detection [2]. These various applications of CNNs suggest the successful application of CNNs for characterizing sprays by image analysis [3]. This work seeks to implement an optical quality control system, capable of assuring that a spray matches some predefined requirements such as the mean droplet diameter $d_{50,3}$ by image recognition.

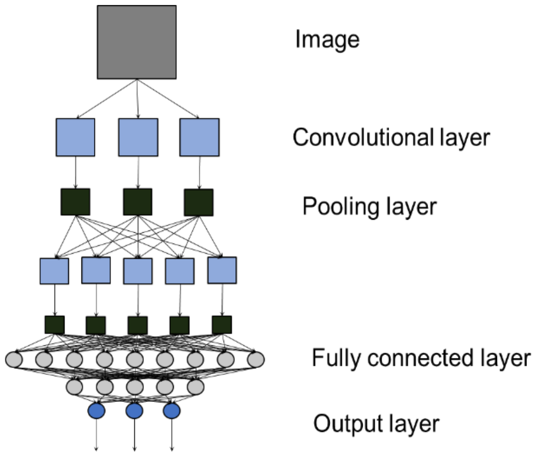

Figure 1: Schematic structure of a Convolutional Neural Network

Material and Methods

A database for the CNN created by operating a commercial nasal spray pump continuously with water using a gear pump (Ismatec BVP-Z 183, Cole-Parmer GmbH, Germany). The drop size distributions of the sprays were measured via laser diffraction (Spraytec STP 5921, Malvern Instruments Ltd., Malvern, UK). For the creation of the image database, the volume flow of the liquid was adjusted in such a way that the generated spray matched the desired value for $d_{50,3}$ for each category. The setup of the image database is represented in Table 1.

Tab.1: Parameters of database for d50, 3 categorization

Category	d50, 3 [µm]	d50, 3, measured [µm]
1	80 – 100	85.8 ± 1.2
2	100 – 120	105.1 ± 1.8
3	120 – 140	132.0 ± 6.3
4	140 – 160	148.0 ± 6.3
5	160 - 180	167.0 ± 5.1

500 images of the spray were taken for each category by a commercially available camera (Nikon Z6 24-70/4 S, Sendai Nikon Corporation, Natori, Japan)). The spray (Figure 2) was illuminated by two LED-spotlights (KL 1600 LED, Schott AG, Mainz, Germany) placed behind the aerosol relative to the camera position.

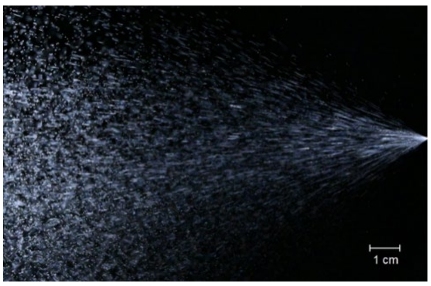

Figure 2. Image taken from the database for $d_{50,3}$ classifications.

The net for the categorization of the $d_{50,3}$ consisted of ten layers in total, three convolutional and pooling layers respectively, one flattened layer to convert the two-dimensional images into a one-dimensional vector and two dense layers. The last layer, the output layer, consisted of five nodes, one for each category.
For the categorization of the drop size distribution, the net architecture had to be adjusted in such a way that the output layer with five nodes was replaced with five parallel output layers with one node each. Due to the high CPU requirement, this architecture resulted in one single classifier consisting of a stack of three dense layers with five independent output layers, one for each drop class of the drop size distribution to be categorized. For this task, the images for determining the $d_{50,3}$ were reused but labeled with the corresponding drop size distribution. This led to five drop size distributions with 500 image examples each. The measured drop size distribution was modified beforehand in such a way that the measured drop classes were assembled into five drop classes to reduce computing power.

Results and Discussion

In order to train the CNNs, the image database consisted of 2500 images in total. 500 images of each category (see Table 1) were in turn split up with 80 % in training data and 20 % in test data. Also, the training data were split up with 70 % data on which the weights were adjusted and the remaining data for validation of the success in the structural change (see Figure 3).

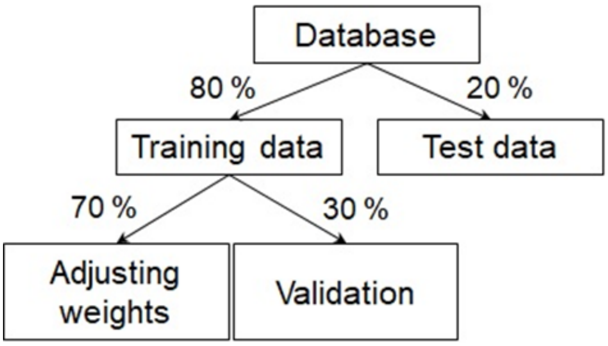

Figure 3. Split up of the database for training, validation, and evaluation purposes.

The adjustment of the weights is based on a loss function representing the deviation of the value given by the CNN on the real value (label) calculated by equation (1) with yi as the labeled value to be assigned, $\hat{y}_i$ representing the CNN value for class i out of n classes.

$$Loss = -\sum_{i=1}^{n} y_i \, ln(\hat{y}_i) \tag{1}$$

The training history for the first of five training runs is represented in Figure 4. Black triangles and dots show the loss function and accuracy over the epochs during adjustment of the weighted connections. Grey triangles and dots represent loss function and accuracy during validation at the end of each epoch.

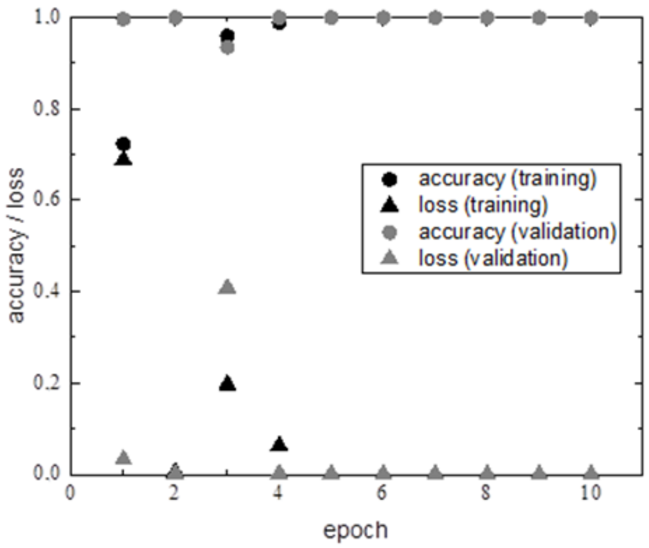

Figure 4. Training history for the first training run for $d_{50,3}$ classification.

Both training and validation loss show a descending trend with an increasing number of epochs reaching a value close to zero after the fourth epoch. The values fit quite well with the real values and in turn, the number of correctly categorized images increases with an increasing number of epochs, as can be seen from both the training and validation accuracy. The five different training runs leading to a different Model with the same architecture of the CNN. Finally, each CNN trained by 2000 labeled images and the training success was evaluated by the certainty of the classification of the test data, which are not a part of the training data. The output of the CNN is a probability distribution over all categories for each image indicating the probability for the image to belong to one class or another. The trained CNNs classified all of the 500 images in the correct drop size classes presented in figure 1.

To not only assign the images to a category of a median drop size with a certain probability but also categorize the values of each drop class of the distribution, the architecture of the network had to be adjusted to this task as described above. The measured drop size distribution was modified beforehand in such a way that the measured drop classes were assembled into five drop classes to reduce computing power. The aim was to give a probability value for each of these five classes by the CNN close to the real value for the corresponding drop class for the five drop size distributions.

The results for two of the drop size distributions are shown in figure 5. The darker bars show the mean of the measured and modified distribution based on 20 measurements done by laser diffraction. The light gray bars show the mean value of the distributions done by the CNN for 500 images for each drop size distribution. Error bars represent the 95 % confidence interval for n = 20 and n = 500 for the measured and distributions given by the CNN, respectively. The low deviations between the values show that it is possible to categorize droplet size distributions via CNNs with a high confidence level for this particular task.

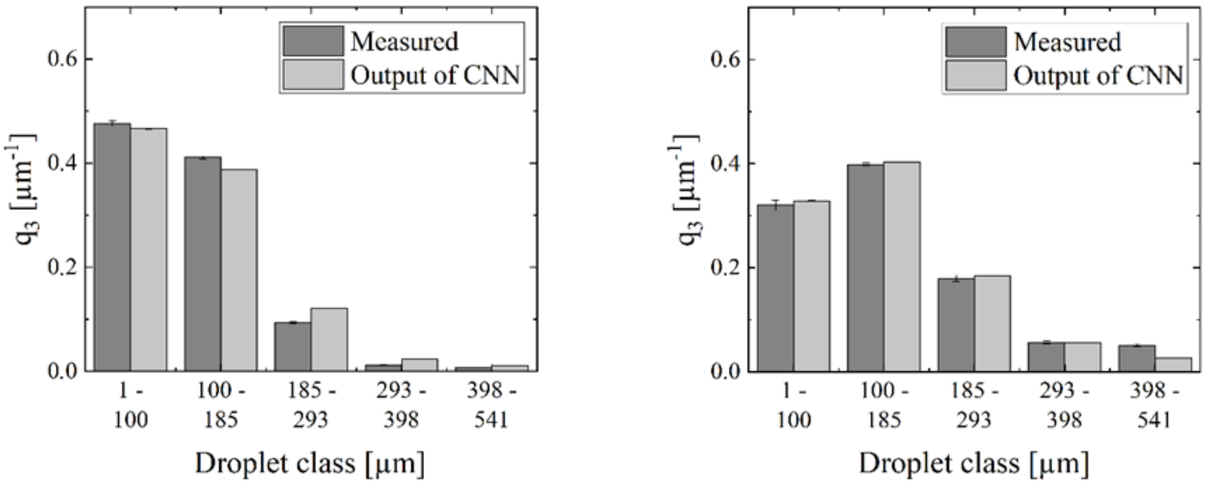

Figure 5. Two out of five investigated drop size distributions.

Conclusions

In the present work, CNNs were used to assign Spray images correctly to spray categories, each represented by a mean droplet diameter ($d_{50,3}$) with a range variation of 20 µm. Moreover, CNNs were successfully trained for the categorization of a drop size distribution consisting of five drop classes. The deviation of the distribution as an output of the CNN from the measured distributions is in a range of 0.1 - 1.5% for each class.

Subsequently, CNNs trained on different tasks can be combined to build up a robust sensor system e.g. for quality control purposes, giving a multi-parameter output to evaluate aerosol quality.

Nomenclature

$d_{50,3}$	volume based median diameter [µm]
y	labeled value [-]
$\hat{y}$	predicted value by the CNN [-]

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