

Material Methods and Technology

2.1. Materials

Metal oxides-based semiconductors have been very common in the gas sensing community, as was covered in Chapter 1. Metal-oxide (MOX)-based gas sensors, unlike other types of gas sensors currently in use, display gas detecting phenomena by altering the electrical characteristics of the sensing materials. These gas sensors offer good selectivity and are less expensive. Three publicly accessible datasets and one dataset that was recorded in the lab of our own department were both used in our published works to date. The gas sensor array made up of MOX-based gas sensors was used to record all of these datasets. It would be helpful to know every detail about MOX gas sensors before talking about these datasets.

2.1.1. Metal oxide semiconductors (MOX) for Gas Sensing

Metal oxide semiconductors exhibit distinct features from elemental semiconductors as a result of the discrepancy in charge carrier transport brought on by the interaction of the metal and oxide orbitals. Because the electrons in metal oxides are more mobile and have smaller effective masses than the holes, carrier transport is enhanced. These n-type conductivity semiconductors, like SnO₂ and ZnO, are made of metal oxides. However, metal oxides can also exhibit p-type conductivity if the holes' effective masses are considerably lower than those of the electrons. Nickel Oxide (NiO), as we discovered in the literature, has been regarded as the first p-type metal oxide semiconductor since 1993 [153]. Cu₂O and CuMO₂ (M = Al, Ga, or In) are other p-type metal oxide semiconductors in addition to NiO [154].

Figure 2.1 shows the Application of MOS-based gas sensors in various fields and their inherent characteristics for developing efficient gas sensors.

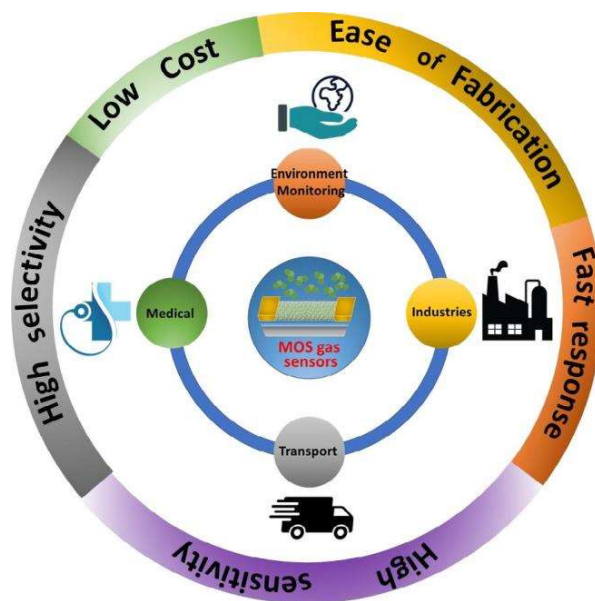


Figure 2.1.Application of MOS-based gas sensors in various fields and their inherent characteristics for developing efficient gas sensors [155]

2.1.2. MOX Gas Sensors: Working

The sensing component is printed on the device's base material in MOX gas sensors. This set-up is positioned above a heater that generates thermal stimulation for the sensor material. A temperature of several hundred degrees Celsius is produced by this heater. The covalent bonds are then disrupted as a result of thermal excitation, resulting in free electrons in the sensing material. These unbound electrons move freely inside the detecting substance and produce a quantifiable current. But when the sensing material is put in a neutral environment, this behaviour happens.

Additionally, the oxygen that is currently present is adsorbed on the sensing material if the detecting device is placed in clean air. The free electrons of the sensing

material are trapped by the adsorbed oxygen, increasing the resistance of the sensing material. The free electron movement is being slowed down by this process. Methane, propane, and other reducing gases and odors react with the adsorbed oxygen on the sensor material when this gadget is exposed to them. In the sensing material, this reaction makes the free electrons that were previously imprisoned by the adsorbed oxygen available once again. It lowers the resistance of the sensing material, allowing more electron movement and a larger current as a result. The amount of exposed gases or odors directly relates to the increase in the flow of free electrons.

2.1.3. Responses of MOX Gas Sensors

As we looked at in the previous subsection, the concentration of the exposed gas or odor directly relates to the change in the sensing material's resistance. We notice this change in resistance to identify the gas. The types of conductivity of the sensing material (n-type or p-type) and the type of exposed gas or odor (reducing or oxidising) determine whether a change in resistance is noticed during the detection of the gas or odor (reduction or rise). However, in each instance, the variation in resistance is related to the gas or odor concentration. Fig. 2.1 depicts a schematic response curve for the MOX gas sensor. The MOX gas sensors measure the electrical characteristics of the sensing materials (resistance, conductance, etc.) to identify the gases/odors.

The sensitivity, selectivity, response and recovery times, stability, detection limit, and optimal operating temperature are some important criteria used in the characterisation of gas sensing. The relationship between response and recovery time contains a wealth of information [156], as seen in Fig. 2.2. The approximate steady-

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state values are shown in the constant portion. Only steady-state responses have been used to categorise and quantify the gases since the invention of MOX gas sensors decades ago. Furthermore, the steady-state responses are regarded as the industry standard for gas sensing [157]. The use of steady-state reactions to categorise the gases in the real-time scenario is constrained because the approximate steady-state is only reached after a significant amount of time. This restriction makes the use of dynamic reactions possible. The dynamic reactions have now entered the picture after many years. High-dimensional data are produced as a result of the dynamic responses being obtained by sampling the response to recovery time curve. It is possible to process the data with less computer resources when the steady-state answers are used. However, the dynamic responses that were collected include both transient and steady-state responses. To prepare a high-dimensional dataset for categorising gases and odors, extra pre-processing processes are needed.

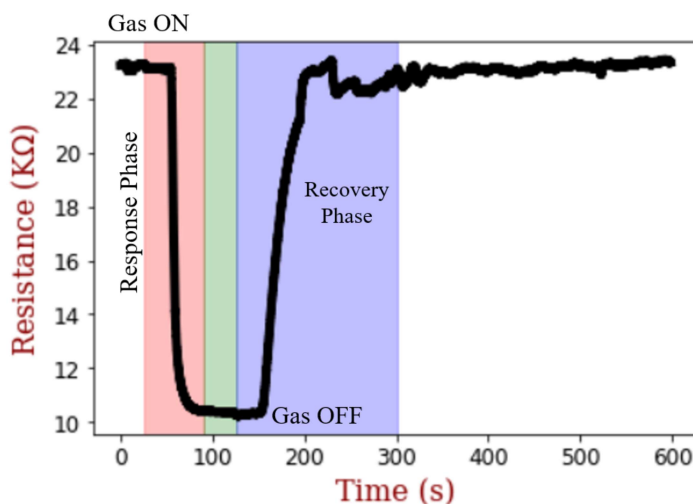


Figure 2.2: Response of a MOX (TGS2610) Gas Sensor for Ethylene at 125 ppm [??]

2.1.4. Steady-State and Sampled Dynamic/Transient Responses

Steady-State Response: Once the gas sensor has reached a steady state, a static value is obtained. As a result, every gas exposure at a specific concentration yields a single-valued data point. To provide a dataset with better steady-state responses for gas analysis, the gas concentration is altered. When a gas sensor array is utilised for gas sensing rather than a single gas sensor, the steady-state response it produces has data points equal to the number of gas sensors in the array. As a result, the acquired steady-state responses include a wealth of information and better describe the sensed gas or gases. As seen in Fig. 2.3, one static value is provided by a single steady-state region for a single gas sensor, but utilising an array of four gas sensors, we may obtain four steady-state values.

Sampled Dynamic/Transient Response: The existence of two transient zones, one in the response phase and the other in the recovery phase, has also been demonstrated in Fig. 2.3. The steady-state is located in the space between these transient zones. There are three ways to gather the datasets when using the gas sensor responses for real-time gas classification:

1. During the sampling of the transient from the response phase.
2. Which types of responses—static and transient throughout the response phase—are sampled?
3. The full responses, from transient during the response phase to transient during the recovery phase, are sampled.

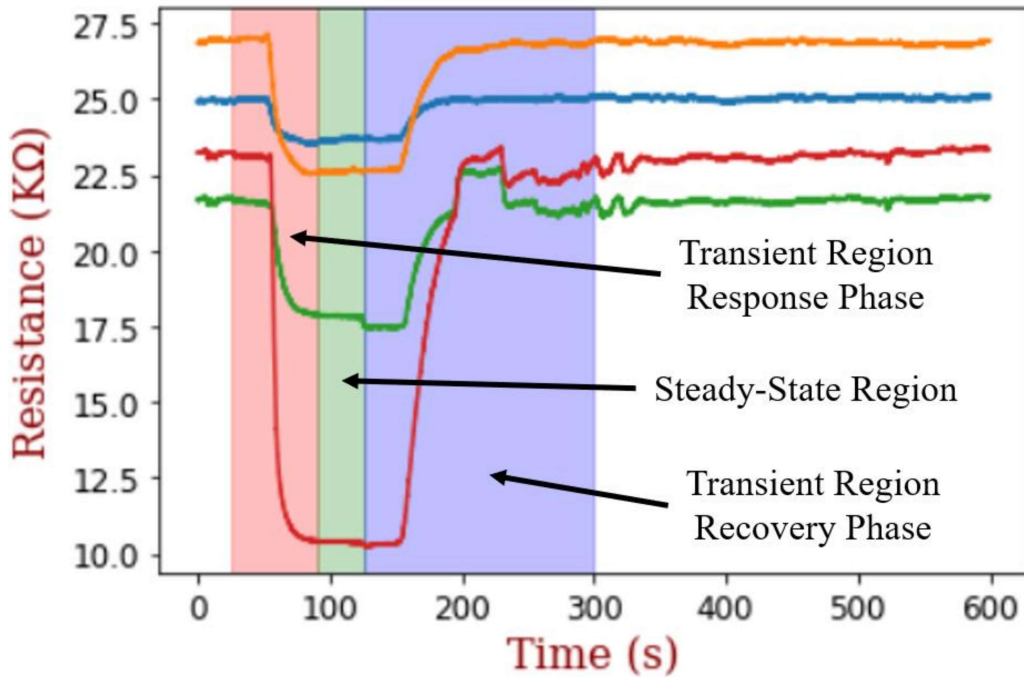


Figure 2.3: The Captured Steady-State and Transient Regions of Ethylene and Carbon Monoxide Sensor Array Responses

The resulting datasets are complicated and high-dimensional. Additionally, the lengthy duration and high sample rate may further grow the data, making it complex and enormous. Such dynamic responses cannot be used to classify gases in the conventional manner because effective data pre-processing necessitates more computational capacity. As a result, but at the sacrifice of computer resources, the transient or mixed responses can be employed to classify the gases in a real-time scenario. In addition, the dynamic responses drift far more than the steady-state responses.

To illustrate the research reported in this thesis, we used four separate datasets gathered from four different arrays of MOX gas sensors. The fourth was recorded in the lab of the department at our own Institute, whereas the other three are accessible

to the public for academic purposes. These datasets have also been thoroughly examined in order to comprehend the modality of each dataset.

2.1.5. Dataset

Using a four-element integrated gas sensor array, this dataset was recorded. It was created with the use of thick-film technology with the intention of analysing the sensitivity and response time. The aforementioned sensing components were created on a basis of tin oxide by doping it with cadmium sulphide, molybdenum oxide, and zinc oxide. The fourth one was utilised to make tin oxide that wasn't doped. This integrated gas sensor array, which was exposed to four gases/odors—acetone, carbon tetrachloride, ethyl methyl ketone, and xylene was used to gather the sensor characteristics [158]. This dataset is divided into two sets, each with 42 and 16 samples. In [159], provide a clear explanation of how these samples were extracted .

2.2. Methods

Data analytics uses a variety of pattern recognition algorithms to categorise and measure gases and odors. However, a number of conventional pattern recognition approaches show promise in particular applications involving the estimation and discrimination of gases and odors. However, because to their wide range of applicability in the context of gas sensor response analysis, neural networks continue to dominate for each task at hand. Additionally, when compared to their competitors, neural networks have minimal constraints for the same applications.

2.2.1. Artificial Neural Networks (ANN)

Traditional artificial neural networks (ANNs) only employ dense or completely linked layers. One-dimensional vector input is needed for these layers.

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Due to their complete connectivity, these layers produce large trainable parameters, which slow down the computational process. Furthermore, such networks only pick up on salient, discriminable features based on linear variance that are fundamentally restricted to 1D vectors. Fig. 2.4 depicts a typical ANN for identifying the gases/odors. The response vector acquired by the gas sensor array is represented by each node in the input layer. Each node in the output layer generates a probability estimate for the target simultaneously. The target with the highest probability estimate is taken into account when classifying the input vector's final targets. The layer between input and output, generally known as the hidden layer, is depicted in Fig. 2.4 and can be employed in numbers as needed, but it creates a complex design. A "perceptron" is a type of mathematical function that is represented by each hidden layer node. As a result, each fully connected layer (hidden layer) is made up of a parallel configuration of perceptrons. Consequently, multilayer perceptron (MLP) networks are another name for ANNs. A schematic diagram of a perceptron is shown in Fig. 2.4.

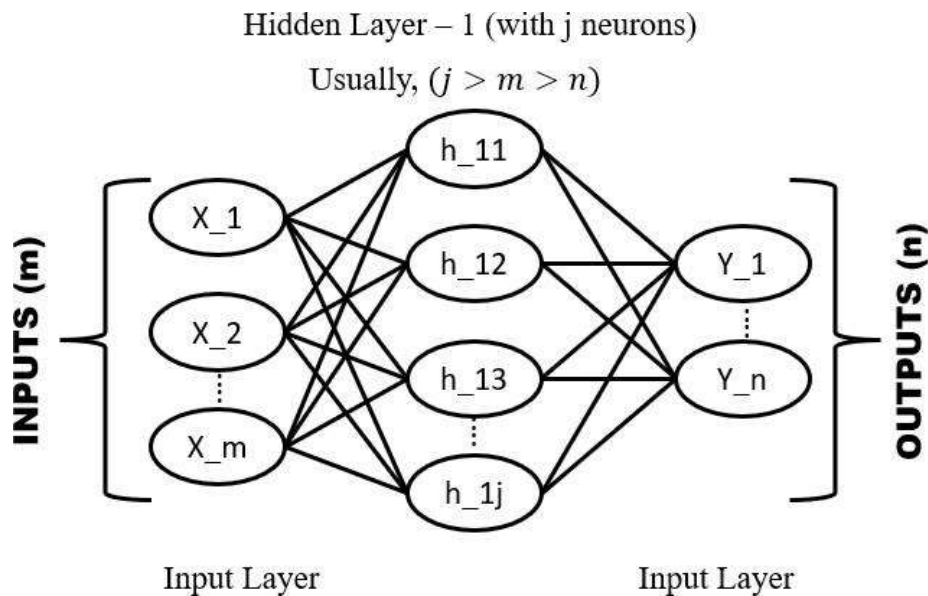


Figure 2.4: General Architecture of Artificial Neural Network

A perceptron, neuron, or the unit cell of neural networks has three parameters in addition to input and output values: weight, bias, and activation function. Weight is a parameter that affects how much the input value is amplified or attenuated. Following some stochastic process, each weight matching to the inputs is created at random. The weighted total of the inputs is employed with these weights as the input to a bounded input bounded output (BIBO) activation function, which produces the perceptron's final output.

To understand the nonlinear relationship between the input and output, activation functions are used. But there isn't a single activation function that works best for every issue. The features it must possess depend on the assignment. Consider the scenario where the weighted total also becomes 0 as a result of all inputs becoming zero owing to noise or another nuisance. In such circumstances, several activation functions cannot be explicitly stated for zero input value. To prevent the circumstance when an activation function receives a zero input value, an offset value (constant) is added to the weighted sum. The Bias is a commonly used value that is normally taken to be 1 (by default). Several activation functions are frequently used by researchers, which are as follows:

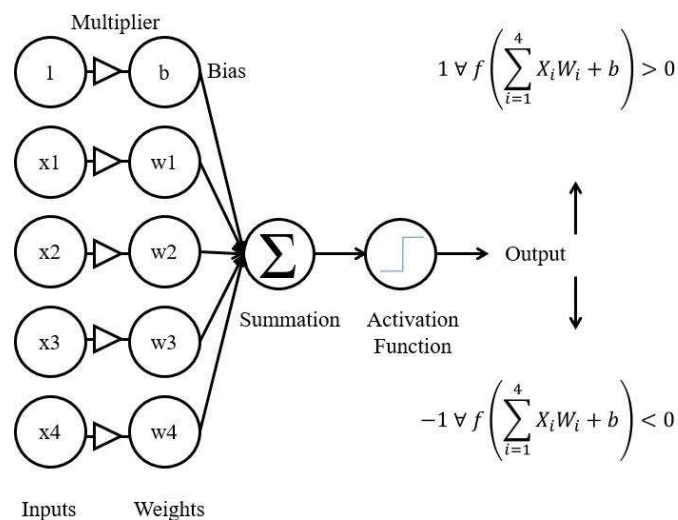


Figure 2.5: Perceptron Architecture

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A linear function is one of the basic activation functions. It cannot use the updated weights and biases to enhance performance due to its continuous gradient and independence from inputs. Therefore, it cannot be used in concealed layers. However, by employing it as an activation function, many single-layered ANNs operate satisfactorily. In output layers where continuous outputs are approximated, linear activation functions are typically utilised. The sigmoid activation function is the most popular. Being continuously differentiable and one of the non-linear functions, it provides a number of benefits. However, the gradient is disappearing, which is an issue. Additionally, sigmoid functions have a range of $[0, 1]$, which is not centred at the origin. It can only generate positive values because it is asymmetrical. It is widely utilised in output layers for binary classification challenges in contrast to these problems. Additionally, the sigmoid activation function's asymmetry problem is solved by the hyperbolic tangent (tanh), which is also a major activation function. It is centred on the origin and spans the range from -1 to $+1$. It is widely employed in hidden layers because of this feature, which makes it excellent for optimisation. However, it also has problems with fading gradients. Rectified linear units (ReLU) are the most often utilised activation function for hidden layers. Compared to the activation functions mentioned above, it is computationally efficient. As was already noted, the output activation function for binary classification is the sigmoid function. For multiclass classification issues, the softmax activation function is effectively employed as the output activation function. For each input and each target, it gives probability estimates. To get over the drawbacks of the discussed activation functions, numerous variations of certain of these activation functions also exist in the literature.

2.2.2. ANN Compatibility with Array Response Modalities

According to what was previously discussed, if the input data vectors are created using the steady-state responses, each vector will contain as many data points as there are gas sensors in the array. According to a review of the literature, a gas sensor array typically consists of 4 to 16 gas sensors. However, there isn't a general rule in the literature for how many gas sensors should be used in an array. This means that a gas sensor array with four gas sensors will only have four data points in its input data vectors. A straightforward ANN is needed to categorise the target gases/odors from these short data vectors.

In contrast, when using transient responses, the resulting input data vectors, which rely on the sampling rate and length, have enormous volumes. It is not advised to use such data vectors directly because doing so would waste computational resources and time. Because a very complicated ANN architecture is needed to process the raw input data vectors as they are. Raw input data vectors may also cause the training model to overfit. In these situations, raw data vectors are pre-processed using a variety of techniques for a variety of goals, including dimensionality reduction, feature selection, feature extraction, etc.

Convolution and pooling layers allowed ANNs to develop into the new paradigm known as deep neural networks (DNNs), which replaced them. The term "deep" is used to indicate two separate things in neural networks: first, that there are more than two hidden layers in ANNs; and second, that convolutional and pooling layers are being used. Convolutional neural networks (CNNs) are a common name for ANNs that use convolution and pooling layers. In the realm of neural networks, the

CNNs have established standards. They have a reputation for having issues with picture classification. The following section goes over how scientists have begun to employ CNNs in the study of gas sensing. We've talked about why we chose to employ CNNs for gas sensing in a brand-new approach that has never been done before.

2.3. Technology Background

With the exception of CNNs, conventional pattern recognition methods, such as ANNs, require 1D data vectors for target classification. Furthermore, these depend heavily on the handcrafted (manually derived) characteristics for superior performance. The issue of feature ranking or selection then arises for these features. The task at hand becomes more computationally difficult when important attributes are determined. When features are manually extracted, a CNN provides the solution to all of these issues. CNN excels because of its capacity to automatically extract high-level features. It is a well-known global technique, as was previously said, that attracted attention from the picture classification challenges. Binary and grayscale images are 2D structures, while colour, multispectral, and hyperspectral images are 3D structures. For instance, the MNIST data, which contains of grayscale photographs of handwritten digits, has been classified using a pioneering CNN [161]. In contrast, CNN has been used to categorise hyperspectral images [162].

Due to its two-dimensional operability for convolution and pooling operation, the original CNN is also known as a 2D-CNN. However, the one-dimensional and three-dimensional forms of it later formed using the contextual outlines. Every CNN variant has relevance, depending on the application, however

2D-CNNs have been more commonly modified to make use of their significance in various contexts. For instance, the first use of a 2D-CNN in the field of gas sensing was published in 2017, and the related works in the field of gas sensing attest to the effective usage of 2D-CNNs for a variety of applications. It might be worthwhile to first go over a 2D-CNN's general design before talking about how it can be used for gas sensing.

2.3.1. A General Architecture of 2D-CNN

CNNs were first intended to handle classification issues by extracting the key features from the 2D input vectors. They are specialised neural network designs. CNNs are computationally efficient when compared to conventional neural networks. Fig. 2.6 depicts the broad and most basic design of a 2D-CNN. It differs from conventional architectures in that it contains two specialised components in the form of convolution and pooling layers.

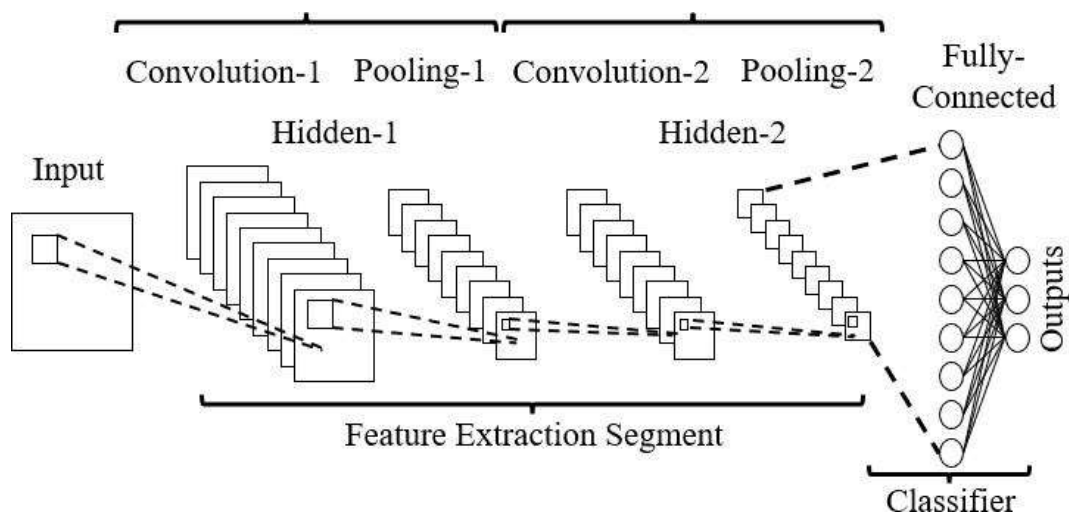


Figure 2.6: A Simplest Architecture of 2D-CNN

The convolution layer is involved in some processes that are used to implement perceptron-like features in ANNs. A filter or kernel (a collection of

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weights) operates on the input data spanning all associated receiving fields in a convolution operation to produce the appropriate feature maps. Fig. 2.7 displays a schematic representation for a 2D convolution operation.

The receptive fields are highly linked when processing images. To minimise the dimensionality and subsequently the trainable parameter, pooling layers are employed to down-sample the generated feature maps. By pooling layers, the architecture becomes computationally effective. The purpose of pooling is to preserve the pooled window's maximum, average, and minimum values. Fig. 2.8 displays a schematic representation for a 2D max-pooling procedure.

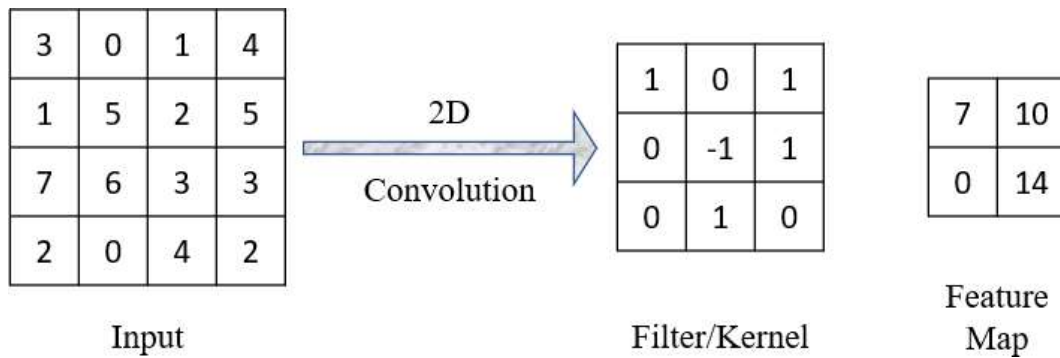


Figure 2.7: 2D Convolution Operation

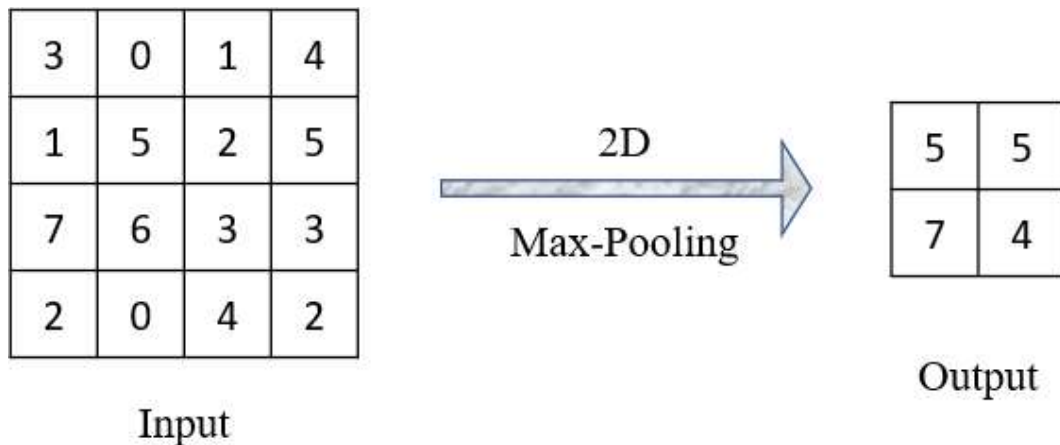


Figure 2.8: 2D Max-Pooling Operation

2.3.2. Motivation for Using 2D-CNN for Gas Classification

The explanation up to this point has made it clear that 2D-CNN was created to operate on 2D data structures, particularly images. With the current state of development, 2D-CNN is used on images in two different ways. A whole image is utilised as the input in the first scenario, while a collection of pixels (or patch) is used in the second scenario. For an example, see Fig. 2.9.

Using the second example, we have utilised 2D-CNN in a number of publications that are not related to the thesis that was just stated [162-165]. In these works, the input used to categorise the targets is a collection of pixels (a patch). These tiny patches have shapes like (5×5) , (7×7) , (9×9) , and so on [161]. They are squared 2D data structures. From this, we have concluded that a small patch with the dimensions (5×5) can be used as the input for a 2D-CNN. A gas sensor array typically consists of 4 to 16 gas sensor components, yielding 4 to 16 data points for each sample captured for each observation, as stated above. In 2D-squared structures with shapes ranging from (2×2) to (4×4) , the generated response vectors can thus be represented. Our response vectors are still incompatible with the 2D-CNN at this size. We have successfully provided specialised data transformation methods to get around this restriction. However, gas sensing has previously used 2D-CNNs since 2017. But for gas sensing, authors and researchers have employed extremely complicated systems. When working with real picture datasets, it is worthwhile to use such extremely complicated designs. In contrast, the data in gas sensing is processed to represent in a 2D format to artificially imitate the real image. Additionally, the 2D-CNNs for gas classification that have been discovered so far can only be used with

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dynamic answers; when only steady-state responses are provided to categorise the gases or odors, they are ineffective. We have also gotten beyond this restriction.

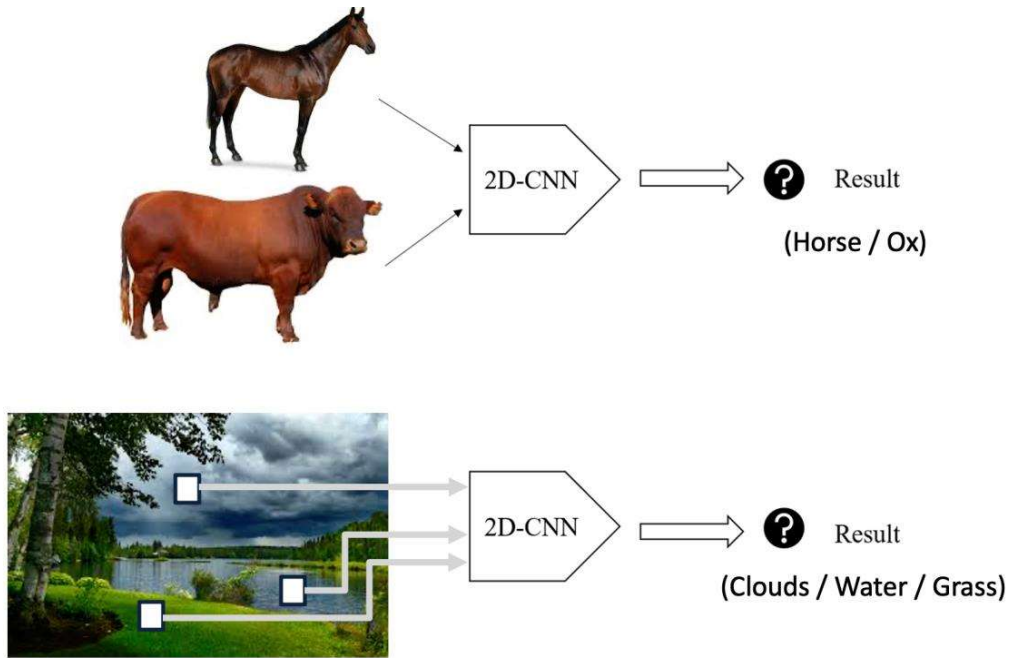


Figure 2.9: Single / Multi-object classification using 2D-CNNs

2.4. Conclusion

A range of technology is available to design gas sensors based on various gas detection principles in the field of gas sensing. In general, the researchers have divided the gas sensors into two categories. One type of gas sensor uses the variation in electrical properties of the sensing materials to detect gases, and another type of gas sensor uses non-electrical qualities. However, the first type of MOX gas sensors is significantly more common in the field of gas sensing research. The MOX gas sensors do not necessarily provide correct service everywhere. The MOX gas sensors provide a number of advantages, including affordability, rapid reaction, longevity, suitability for miniaturisation, etc. It also has a number of drawbacks, including poor selectivity,

drifting responses, and a strong dependence on humidity and temperature. However, the combination of a MOX gas sensor-based array with cutting-edge pattern recognition methods is setting new standards for gas sensing. The responses from MOX gas sensors have been utilised to classify the gases/odors using nearly all pattern recognition algorithms. However, neural networks have dominated the field for many years. ANNs are typically used to categorise gases and odors, but these networks only have fully connected layers, which limit the amount of training parameters that can be employed. The complexity of neural networks decreased with the development of advanced convolutional and pooling layers. These layers provide sparse connectivity and parameter sharing to conventional topologies. Additionally, ANNs are used to enhance the features of data that has been manually processed. However, the convolutional neural networks that make use of the convolution and pooling layers have the ability to automatically extract high-level features and deliver superior outcomes.

We have modified the convolutional neural networks popular for image classification for gas sensing based on this reasoning. We have suggested specialised data transformation strategies that make the gas sensor responses compatible with 2D-CNN because the responses from gas sensors are naturally available in 1D vectors. Additionally, using the dynamic and static responses from the gas sensor array, we have created a 2D-CNN that is simpler and is capable of differentiating gases and odors. We do not employ pooling layers in the customised CNN because they are only necessary when utilising CNNs for image classification. However, pooling layers may make use of their relevance for non-imaging datasets that are extremely complicated and highly linked. With our customised CNN, we have contributed in a novel way to

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the use of CNN for the classification of gases and odors independent of the modalities of response from gas sensor arrays. Additionally, we have suggested an optimisation strategy for gas sensor nodes that is suitable for environments with limited resources. Additionally, we have developed a hybrid CNN architecture that can account for drift effects without the need for extra statistical algorithms.