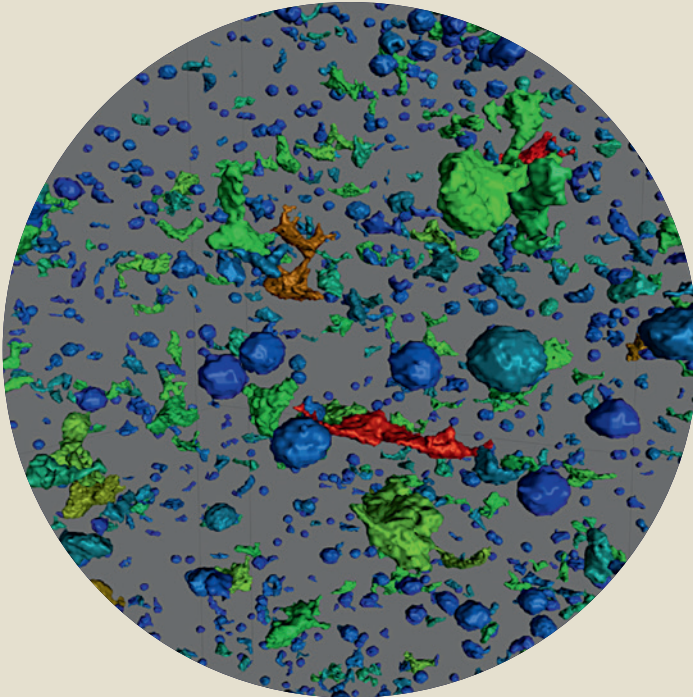




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Natan Nudelis

Machine Learning for Additive Manufacturing and Hot Isostatic Pressing based on Quality Characteristics

Machine Learning for Additive Manufacturing and Hot Isostatic Pressing based on Quality Characteristics

Natan Nudelis

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Abstract / Kurzfassung

Additive manufacturing (AM) using laser powder bed fusion (PBF-LB/M) has many advantages such as design freedom and sustainability. However, AM also suffers from internal defects that limit its functionality. Furthermore, post-treatment methods like hot isostatic pressing (HIP) promise to enhance material properties. This work aims to develop a machine learning model using artificial neural networks, to predict PBF-LB or HIP process parameters based on quality characteristics.

Additive Fertigung (AM) mittels Laserstrahlschmelzen (PBF-LB/M) bietet viele Vorteile, wie Designfreiheit und Nachhaltigkeit. Jedoch leidet AM unter internen Defekten, die seine Funktionalität einschränken. Nachbehandlungsmethoden wie das heißisostatische Pressen (HIP) versprechen eine Verbesserung der Materialeigenschaften. Ziel dieser Arbeit ist es, ein maschinelles Lernmodell für die Vorhersage von PBF-LB/M oder HIP-Prozessparameter unter Verwendung von Qualitätsmerkmalen zu entwickeln.

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Abbreviations

Al	Aluminium
AM	Additive Manufacturing
ANN	Artificial Neural Network
AUC	Area under the ROC Curve
CoD	Coefficient of Determination
CT	Computed Tomography
DIN	Deutsches Institut für Normung
EN	Europäische Norm
e.g.	For example
FEA	Finite Element Analysis
FN	False Negative
FP	False Positive
FPR	False Positive Rate
HIP	Hot Isostatic Pressing
ISO	International Organisation for Standardisation
PBF-LB/M	Powder Bed Fusion – Laser Beam/ Metals
MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
MCC	Matthews Correlation Coefficient
MSE	Mean Squared Error
MSW	Mean Squared Weights
ML	Machine Learning
MLP	Multilayer Perceptron
OVA	One-vs-All
OVO	One-vs-One
RL	Reinforcement Learning
RMSE	Root Mean Squared Error
ROC	Receiver Operating Characteristic
SL	Supervised Learning
SLP	Single Layer Perceptron
SLM	Selective Laser Melting
SOM	Self-Organising Maps
TN	True Negative
TP	True Positive
TPR	True Positive Rate
UL	Unsupervised Learning
VED	Volume Energy Density
XOR	Exclusive OR

1. Introduction

Additive manufacturing (AM) using laser powder bed fusion (PBF-LB/M) offers great opportunities in terms of flexibility, design freedom, reduction of material waste and many more [1,2]. The ability to produce near-net-shape components is of great interest in a variety of industries, including automotive, aerospace and healthcare. Despite these benefits, internal defects such as pores limit the functionality of AM parts. As a result of these limitations, large-scale industrial acceptance of laser powder bed fusion has not been fully achieved yet.

Previous research has focused extensively on investigating the types and origin of defects in the PBF-LB/M process [3–8]. However, porosity appears to be the inevitable by-product of the current state of laser powder bed fusion of Al alloys. Therefore, post-treatment technologies that deal with the removal of pores have been widely used in the field of AM. Hot isostatic pressing (HIP) is a densification process involving the simultaneous application of high-pressures and elevated temperatures. Today, hot isostatic pressing of additive manufactured components is recognised for its ability to produce highly dense and microstructurally homogeneous parts [9–14]. Another critical limitation of AM is the high cost of qualifying the process for industrial applications. The AM qualification process takes a long time due to multiple iterations consisting of sample fabrication and evaluation. Quality constraints or long development times should no longer be an obstacle to product innovation. Fast quality prediction based on manufacturing parameters offers the possibility to overcome these obstacles and make AM even more individual and economical.

In addition, quality is not an absolute value, but is defined relatively according to customer requirements and the intended use. For example, prototypes have different quality requirements than functional components, which means that quality needs to be as flexible as AM production already is. There are many human or process-related influences that affect component quality [15]. This is why physical laws or mathematical equations cannot produce a quality prediction model. Machine learning does not work according to any laws of nature; it uses the information in existing data to learn its behaviour.

The aim of this work is to develop machine learning (ML) systems for predicting PBF-LB/M and HIP process parameters based on quality characteristics such as pore types, part densities or hardness values. Therefore, a supervised machine learning application focused on neural networks needs to be trained with as much

relevant information as possible. The challenge is to find appropriate data that contains enough information about the PBF-LB/M and HIP process using ALSi10Mg. This requires a comprehensive process analysis and the development of appropriate data acquisition methods.

For this reason, the content of this work is divided into two chapters. The first chapter deals with the data preparation and analysis, which has been published in peer-reviewed publications [16–18]. These peer-reviewed articles form the basis of this publication-based thesis. The second chapter focuses on the application of machine learning, which extends the research beyond the included publications. Chapter 2 initiates the explanation of the technical and methodical foundations required for a thorough understanding of the thesis, with a particular emphasis on machine learning. The fundamentals of PBF-LB/M and HIP can be extracted from the underlying publications. The third chapter introduces the objectives and approach, followed by the applied methodology in chapter 4. The contents of the underlying publications are briefly summarized in chapters 5 to 7, followed by the machine learning results in chapter 8. Each of the publications and the machine learning chapter include a comprehensive discussion, which complement each other. The dissertation concludes in a summary where the scientific contribution of this publication-based work is reflected on the basis of the three underlying publications and the machine learning results in relation to the state of the art.

2. State of the Art

2.1. Laser Powder Bed Fusion (PBF-LB/M)

Laser powder bed fusion (PBF-LB/M) is an additive manufacturing process for metallic materials that has received a lot of attention from industry in recent years. This is due to many advantages such as high flexibility, the ability to create complex geometries, cost and waste reduction, and many more [1]. PBF-LB/M machines are typically filled with a gas such as argon, nitrogen or helium to avoid oxidation during the manufacturing. In the first step of the process, the metal powder is applied to the substrate using a coater. In the next step, the laser begins to expose the powder surface according to the geometry specifications from the 3D model. The building plate is then lowered by the set layer thickness and the process is repeated until all the layers of the components have been produced. The PBF-LB/M process uses the thermal energy of a laser beam to melt powder particles, which then solidify and build up the component layer by layer. Figure 1 illustrates the PBF-LB/M process, including key process parameters and material properties.

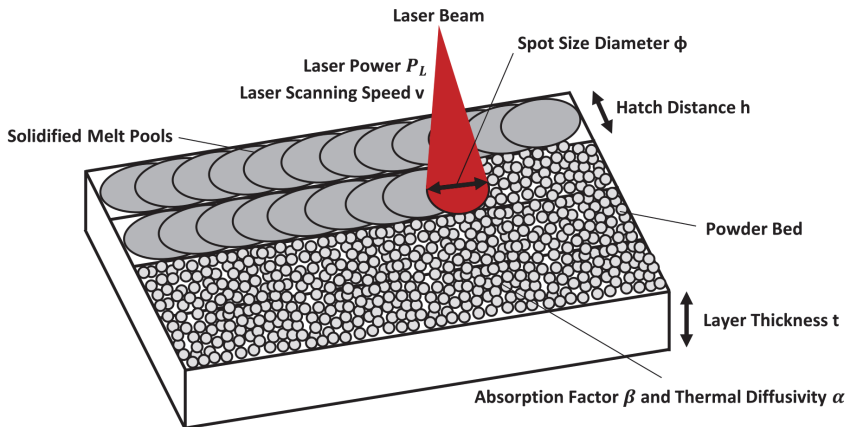


Figure 1: PBF-LB/M process, including the key process parameters and material properties

The melting process can be described by the volumetric energy density (VED) induced in the deposited metal powder. The classical definition of VED is described as the ratio between the laser power P_L (W) and the product of the layer thickness t (mm), the laser scanning speed v (mm/s) and the hatch distance h (mm) [19–21]:

$$VED = \frac{P_L}{t h v} [J/mm^3] \quad (2.1)$$

In addition, a modified definition of VED is given by Ferro et al. [22], which includes the material properties (absorption factor β and thermal diffusivity α) as well as the influence of the spot size diameter ϕ (mm):

$$VED_{modified} = \frac{P_L \beta}{h \sqrt{4\alpha\phi v}} [J/mm^3] \quad (2.2)$$

2.1.1. Pores in AlSi10Mg Components

For PBF-LB/M processes, the evaluation and analysis of porosity has proven to be a valuable tool in determining component quality. Previous research has focused extensively on investigating and explaining the types of pores present in PBF-LB/M parts [3-8]. Three types of pores have been identified as the most common. These pore types can be categorised into spherical and irregularly shaped classes. Hydrogen induced pores and keyhole pores can be distinguished by their spherical shape. In contrast, the so-called lack-of-fusion pores have a highly irregular shape. In addition to influencing mechanical properties, the pore type can also provide detailed information about the process conditions. Many previous research reports on optimising the PBF-LB/M process using AlSi10Mg [4,6,19–21,23] to avoid porosity have been published. The pore shapes, formation mechanisms and quality influences of hydrogen, keyhole and lack-of-fusion pores are further described in the underlying publications I, II, III [16–18]. Overall, these types of pores can have a significant influence on the mechanical properties of the final component and it is therefore important to reduce their formation during the PBF-LB/M process. This can be achieved by optimising the process parameters, or by implementing post-processing techniques such as hot isostatic pressing (HIP).

2.2. Hot Isostatic Pressing (HIP)

Hot isostatic pressing (HIP) is a heat treatment process used to densify material by the simultaneous application of high-pressure and elevated temperatures. It is typically used to remove internal defects such as pores and cracks to achieve part densities approaching 100 %. Other applications include powder densification, diffusion bonding or sintering of metallic or ceramic components. The gas pressure acts uniformly in all directions, resulting in isotropic component properties. Today, hot isostatic pressing of additive manufactured components is acknowledged for creating parts with high density and consistent microstructural characteristics [9–14].

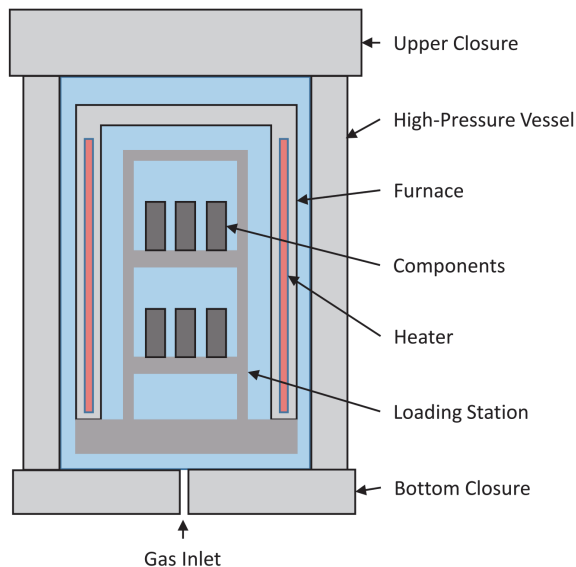


Figure 2: Schematic HIP layout of the high-pressure vessel, furnace and loading station

Figure 2 shows the schematic layout of the high-pressure vessel, including the furnace and component loading station. In terms of safety, the high-pressure vessel is one of the most important components of the HIP system [24]. The pressure vessel is usually filled with an inert gas (e.g. argon), which is used to achieve the high-pressure and to prevent oxidation of the components. The gas atmosphere is also responsible for accurate heat transfer by using the natural convection of the gas. The upper closure seals the system to the outside. Inside the high-pressure vessel lies the furnace, which consists of heating elements and an insulation

mantle. Inside the furnace is the loading station for the components. Both the furnace and the loading station are movable to allow the components to be placed inside the high-pressure vessel. The main process parameters are pressure, temperature and dwell time of the HIP cycle.

2.3. Machine Learning – Artificial Neural Network (ANN)

Machine learning algorithms owe their success in many fields to their ability to learn from available data sets. For instance, speech recognition uses a data set of sound waves, while an autonomous car uses a data set of images to train its ability to recognise the environment. This chapter briefly introduces the concept of labelled and unlabelled data, as well as the most prominent learning methods. Subsequently, the focus is shifted to neural networks, the machine learning method to be utilized in this work.

2.3.1. Types of Machine Learning

Machine learning algorithms can be broadly classified into supervised, unsupervised and reinforcement learning algorithms. In supervised learning (SL), the given data set contains the set of outputs for a set of inputs. The input and output data already exist as typical human-labelled data, which can be used as a set of training samples. The supervised algorithm has to learn the characteristics within the given samples and must create a model that can be used to represent new samples. The most popular supervised learning algorithms are linear regression, support vector machines, k-nearest neighbours, decision trees, neural networks and many more. In contrary to supervised learning techniques, unsupervised learning (UL) is self-organising. A labelled data set is not available. Therefore, unsupervised learning algorithms try to identify trends of similarity in the data and create groups or clusters. Typical unsupervised learning algorithms are clustering (e.g. k-means) and neural networks (e.g. self-organising maps (SOMs)). Finally, reinforcement learning (RL) must be introduced separately from supervised and unsupervised methods. RL algorithms do not have a set of labelled data for training. The data is collected continuously through the interaction with the environment. The comparison between the environmental feedback and the desired behaviour provides the data for training. [25–27]

In this work, the emphasis will be on supervised machine learning methods using the concept of artificial neural networks (ANN).

2.3.2. A Single Neuron – Perceptron

An artificial neural network (ANN) consists of many artificial neurons inspired by the biological setup observed in the brain. The beginnings of artificial neurons can be traced back to W.S. McCulloch and W. Pitts [28]. They presented a simplified model of neural networks, capable of solving logical and arithmetic functions. An important step forward was made by Rosenblatt [29–30] with the invention of the perceptron.

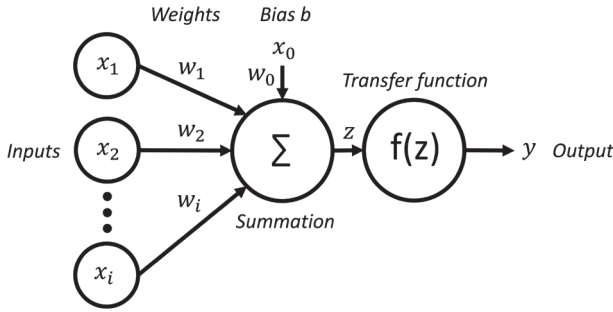


Figure 3: Illustration of a perceptron including bias and transfer function

The perceptron represents the basic unit (neuron) of a neural network (Figure 3). A single-layer perceptron consists of n -dimensional input values $(x_1, x_2, \dots, x_n)$, n -dimensional weights $(w_1, w_2, \dots, w_n)$ and a bias. Furthermore, the weighted sum and the transfer function (activation function) play an important role. The perceptron works by taking numerical inputs (x_n) , as well as the bias, which is a threshold that the perceptron must reach before the output is produced. The bias term acts as an additional model parameter and is represented by an input x_0 and its weight w_0 . Each input value is multiplied by a weight (parameter) that represents the strength of the connection between the units. The weight decides about the influence of the input on the output. The products of input and weight, as well as the bias are then summed up.

$$b = w_0 x_0 \quad (2.3)$$

$$z = \sum_{i=1}^n w_i x_i + b \quad (2.4)$$

The transfer function takes the input z and returns the output y :

$$y = f(z) \quad (2.5)$$

2.3.3. Transfer Functions

The transfer function $f(z)$ is used to normalise the input to a finite range of values. This helps the neural network to recognise patterns and trends in the data set. Many transfer functions can be used for this purpose. Some are shown in Table 1.

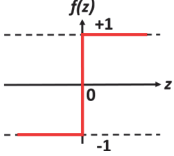
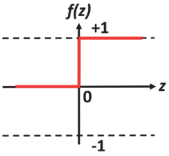
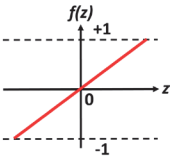
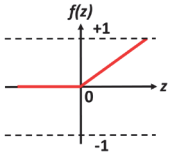
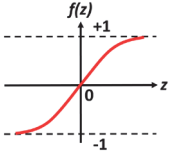
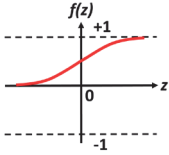
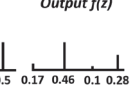
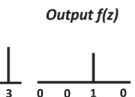
Symmetric hard-limit transfer function		Hard-limit transfer function	
	$f(z) = \begin{cases} -1: & z < 0 \\ +1: & z \geq 0 \end{cases}$		$f(z) = \begin{cases} 0: & z < 0 \\ 1: & z \geq 0 \end{cases}$
Linear transfer function		Positive linear transfer function	
	$f(z) = z$		$f(z) = \begin{cases} z: & z \geq 0 \\ 0: & z < 0 \end{cases}$
Tan-Sigmoid transfer function		Log-Sigmoid transfer function	
	$f(z) = \frac{2}{1 + e^{-2z}} - 1$		$f(z) = \frac{1}{1 + e^{-z}}$
Softmax transfer function		Compet transfer function	
Input z  Output f(z) 	$f(z) = \frac{e^z}{\sum_{j=1}^n e^z}$	Input z  Output f(z) 	$f(z) = \begin{cases} 1: & \max(z) \\ 0: & z < \max(z) \end{cases}$

Table 1: Transfer functions. [31]

For example, the hard-limit transfer function limits the output of the neuron to either 1 if the input is greater than or equal to 0, or the output is 0 if the input is less than 0. The hard-limit transfer function can be used in a single-layer perceptron (Figure 4) to solve linearly separable classification problems. Another example, the log-

sigmoid transfer function, takes the input (any value between plus and minus infinity) and provides the output in the range of 0 to 1. Due to the fact that sigmoid transfer functions are differentiable, they are often used in multilayer back propagation networks (more in chapter 2.3.4). [31]

2.3.4. Network Architecture and Training

The single-layer perceptron (SLP), also called a single-layer neural network, is the simplest feedforward network, consisting of an input and an output layer with no hidden layers (Figure 4). In 1969, Minsky and Papert [32] pointed out that it was impossible for SLPs to solve even an exclusive-or (XOR) problem. Rosenblatt's perceptron (chapter 2.3.2), which uses a hard-limit transfer function, is only capable of solving linearly separable classification problems. This means that single-layer perceptrons without additional hidden layers can't perform non-linear classification.

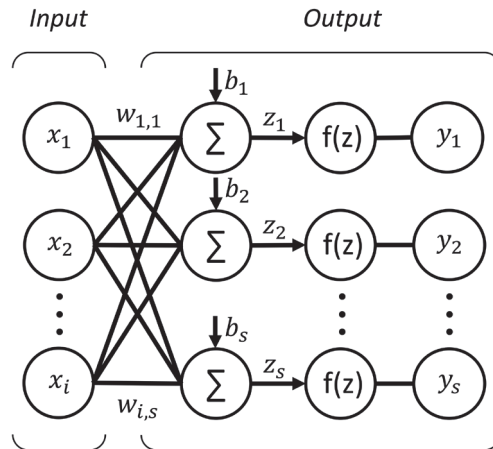


Figure 4: Single-layer neural network

A multi-layer perceptron (MLP), also called a multi-layer neural network (Figure 5), seems to be the logical extension of a single-layer perceptron. One obvious difference is that it is fully connected. Each of the internal neurons is now connected to the neuron in the next layer. Moreover, the number of neurons in all layers (except the first layer) is independent of the input or output dimensionality. This means that the number of neurons in all layers can have any value. It is also worth noting that

single-layer perceptrons and multi-layer perceptrons are mathematically equivalent as long as a linear mapping is used. Therefore, the use of non-linear transfer functions is mandatory. [26]

An important step in training a neural network is the calculation of the error (or loss function). The loss function for a single-layer neural network can be easily calculated as a direct function of the weights and allows gradient calculation. For multi-layer networks, the loss calculation becomes complicated because many layers of weights influence each other. [33]

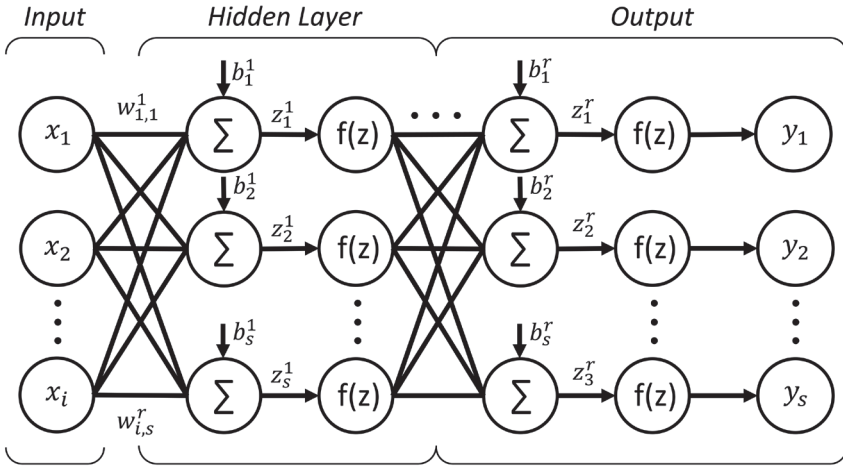


Figure 5: Fully connected feed forward neural network with a single hidden layer (multi-layer neural network)

Therefore, one of the most important multi-layer network architectures is the backpropagation network. The learning process of backpropagation and its general use in neural networks was presented and described in Rumelhart et al. [34]. Backpropagation is a widely used method for training feedforward neural networks [35].

In backpropagation networks it is necessary to calculate the derivatives of any transfer function. The tan-sigmoid, log-sigmoid and linear functions are differentiable and are the most commonly used transfer functions for backpropagation (Table 1). However, other differentiable transfer functions can be used as well. [31]

The backpropagation algorithm calculates the error gradient as the sum of local gradients over different paths to the output node using the chain rule. As a direct application of dynamic programming, backpropagation consists of a forward and a backward phase. First, the forward phase takes the input data and computes the output values and derivatives at various nodes using the current set of weights. The derivatives of the loss functions are computed by comparing the output result with the training instance. Secondly, the backward phase is required to learn the gradient of the loss function with respect to the different weights using the chain rule. These gradients are used to update the weights. [33]

A multi-layer neural network with two or more hidden layers is called a deep learning network [36]. An illustration of a deep learning network is shown in Figure 6.

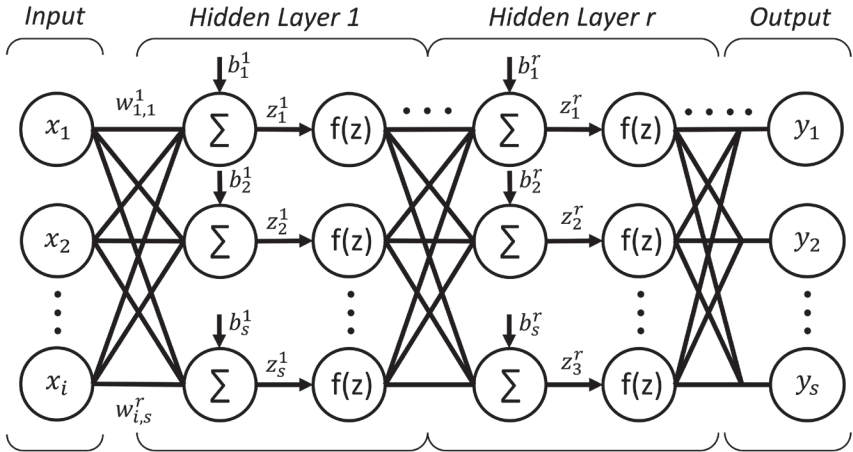


Figure 6: Fully connected feed forward neural network with multiple hidden layer (deep learning network)

2.3.5. Classification Types and Data Format

There are many possible types of classification in supervised machine learning applications. A binary classifier has to decide whether the data belongs to a class or not. There are only two possible choices/ classes. On the other hand, in multi-class classification, the classifier has to choose between more than two classes and the data has to be assigned to only one class. The third type is called multi-label classification. This classifier has to choose between more than two classes, but the data can be assigned to more than one class. [37]

For a better understanding, all three types of classification are illustrated in Figure 7.

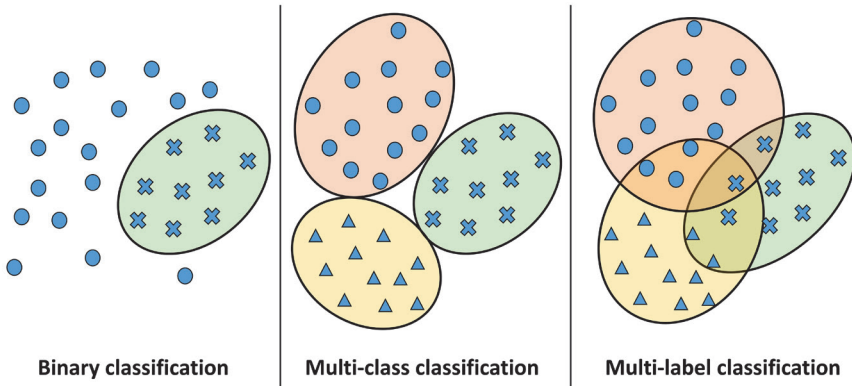


Figure 7: Types of classifications in supervised machine learning

Note that the treatment of categorical features (classification tasks) is completely different from that of numerical features (regression tasks). The data preparation approach for categorical features is called one hot encoding. All classes are represented as 0 or 1. The integer representation is removed and a new binary format is added. The length of the vector is equal to the number of classes. So there is only a 1 in the whole vector (the rest is 0). For multi-label classifications, each possible class is represented by a 1. The problem with integer classes (e.g. 1–7) compared to binary format (0, 1) is the relationship between two numbers. For example, the number 1 is closer to the number 2 than to the number 3, and so on. But classes are not meant to be comparable, like integers. All classes have their own meaning and cannot be compared, which is why, one hot encoding is mandatory for classification tasks. [26]

2.3.6. Class Binarisation

Many research reports have been published on the topic of class binarisation [38–40]. The basic idea is to divide the multi-class data set into binary subsets. The most popular strategies are known as one-vs-one (OVO) and one-vs-all (OVA) classifications [41]. These strategies are designed to reduce many multi-class problems. Multi-class applications are more complex to solve than binary problems. Furthermore, the interpretation of binary classification results is easier than for multi-class classifications. Another problem of many real-world data sets is called class imbalance and deals with a disproportion of class examples. This means that in any data set with an imbalanced class distribution, the minority class is represented much less than the majority classes. This can lead to a poor ability of the model to predict these minority classes. Therefore, class binarisation techniques can be very useful to overcome the problem of imbalanced data [41].

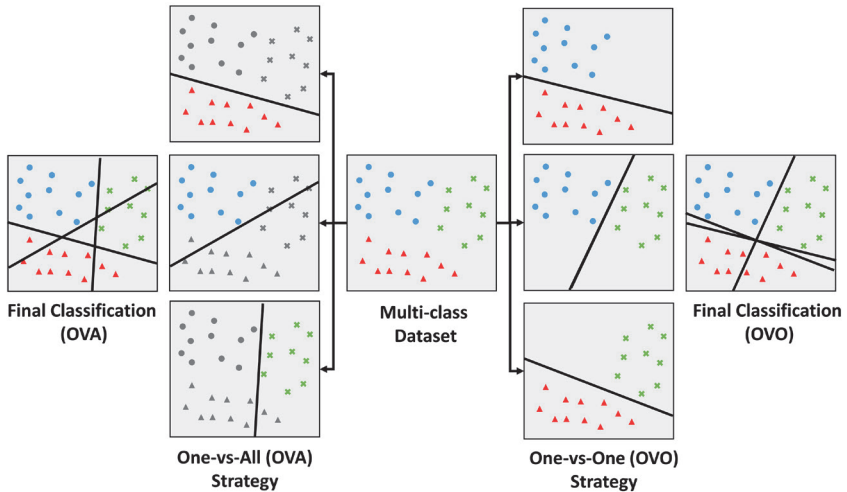


Figure 8: Illustration of class binarisation strategies (one-vs-all (OVA) and one-vs-one (OVO))

An illustration of the OVO and OVA classification strategies is shown in Figure 8. In the OVO strategy, the multi-class data set is split into two-class problems. There are exactly as many splits as there are class pairs. Thus, an m -class problem would be divided into $m(m-1)/2$ binary sub-problems. Each of these sub-problems is trained and validated separately with its own classifier. On the other hand, the OVA strategy also divides an m -class problem into m binary problems. Each sub-problem has its own classifier that distinguishes one of the classes from all other classes. The outputs of each one-vs-one classification can be organised by means

of a score-matrix R^M (Equation 2.6), where $r_{ij} \in [0,1]$ represents the confidence of the classifier discriminating classes i and j in favour of the former. The confidence for the latter is calculated by $r_{ji} = 1 - r_{ij}$.

In the special case where the classifier provides both confidence levels, they have to be normalised so that $r_{ij} + r_{ji} = 1$. Finally, the output from the score matrix can be defined using different aggregation models. For example, the weighted voting strategy can be used, where the confidences are aggregated class by class (by row). The largest sum of confidences will be predicted. [38,41]

$$R^M = \begin{pmatrix} - & r_{12} & \cdots & r_{1m} \\ r_{21} & - & \cdots & r_{2m} \\ \vdots & & & \vdots \\ r_{m1} & r_{m2} & \cdots & - \end{pmatrix} \quad (2.6)$$

On the other hand, the output for each one-vs-all classification can be also organized using the confidence of the classifiers. The class is predicted by the classifier with the highest confidence. The confidences can be summarised in a score vector R^V (Equation 2.7). [38,41]

$$R^V = (r_1, r_2, \dots, r_i, \dots, r_m) \quad (2.7)$$

2.3.7. Hyperparameter Optimisation

In machine learning algorithms, there is a distinction between parameters and hyperparameters. All parameters that the algorithm tunes according to the given data set are called parameters. The algorithm tunes the parameters automatically, without any interaction with the user. All parameters that are based on properties such as the data characteristics or the capacity of the learning algorithm are called hyperparameters. Hyperparameters are set manually before training starts. In the case of a neural network algorithm, all weights and biases are parameters. This is due to the fact that the modelling algorithm decides automatically during the learning process based on the data set. On the other hand, the number of layers, the number of neurons (nodes) in each layer, the batch size, the activation and loss functions (and many more) are hyperparameters and still the choice of the user. Defining the architecture of a neural network is one of the most challenging tasks, which is why there are numerous hyperparameters optimisation methods to facilitate the choice. [42]

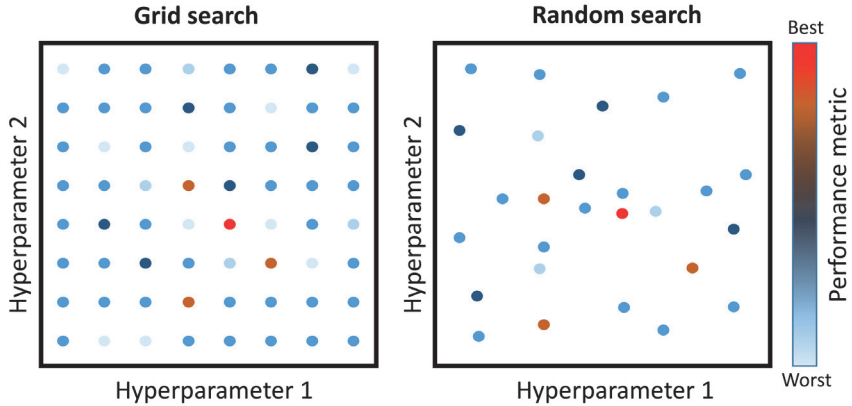


Figure 9: Hyperparameter optimisation approaches

The first approach to hyperparameter optimisation is called grid search (Figure 9). It is the safest way to find the best set of hyperparameters by training the data set on every possible combination. Grid search is a good solution for a manageable number of hyperparameter variations. Otherwise, the training time for each possible combination would be very long (especially for a large data set). The second approach to hyperparameter optimisation is called random search (Figure 9). This method randomly selects hyperparameters and trains the model on them. Using random search can save an enormous amount of time and also find a near best set of hyperparameters. In summary, it depends on the computational effort whether to use the grid search or the random search approach. There are also some more complex optimisation algorithms that are able to keep a log of all the observations and learn from them. For example, the Bayesian optimisation method can solve very complex applications with a huge amount of data and hyperparameter variations. [42]

2.3.8. Performance Metrics

Supervised learning methods can be divided into regression and classification algorithms. The main difference between regression and classification algorithms is the type of the output data. Regression algorithms are used to predict continuous values (e.g. age), whereas classification algorithms are used to classify discrete values (e.g. true or false). All machine learning models, whether classification or a regression, require a metric to judge their performance. The type of output data (continuous or discrete values) determines which performance metrics are used.

In terms of machine learning, the goal is to ensure that the predicted outcome matches the real outcome. The closer the model matches the real outcome, the lower is the error of the model. Botchkarev [43] gave a good overview of performance metrics to measure the error of machine learning regression algorithms. Some of the most commonly mentioned metrics are:

Mean Absolute Error (MAE):

$$MAE = \frac{\sum_{j=1}^n |A_j - P_j|}{n} \quad (2.8)$$

Where A_j represent the actual values and P_j the predicted values. Furthermore, n is the size of the data set.

Mean Squared Error (MSE):

$$MSE = \frac{\sum_{j=1}^n (A_j - P_j)^2}{n} \quad (2.9)$$

Root Mean Squared Error (RMSE):

$$RMSE = \sqrt{\frac{\sum_{j=1}^n (A_j - P_j)^2}{n}} \quad (2.10)$$

Mean Absolute Percentage Error (MAPE):

$$MAPE = \frac{100}{n} \sum_j \frac{|A_j - P_j|}{|A_j|} \quad (2.11)$$

Coefficient of Determination (CoD) or R^2 (R-squared):

$$CoD = 1 - \frac{\sum_{j=1}^n (P_j - A_j)^2}{\sum_{j=1}^n (A_j - \bar{A})^2} \quad (2.12)$$

Where $\bar{A}$ is the mean of the actual values. Unlike the error metrics above, the higher the CoD the better the performance of the model.

In the field of supervised machine learning, especially for classification problems, the confusion matrix is used as a technique to summarise the performance of a classification algorithm [44–48]. An illustration of a confusion matrix is shown in Figure 10. The matrix shows the number of correct and incorrect predictions, represented by different classes (True Positive (TP), False Positive (FP), False Negative (FN), True Negative (TN)). Thus, the matrix provides insight not only into the errors being made, but also into the types of errors. TP represents the cases where the predicted value is positive and it's correct. FP is the number of times the model incorrectly predicted negative values as positive. TN represents the cases where the predicted value is negative and it's correct. The last error class is FN and is the number of times the model incorrectly predicted positive values as negative. The confusion matrix can be used and evaluated for binary or multi-class problems.

		Actual	
		Positive (0)	Negative (0)
Predicted	Positive (1)	TP	FP
	Negative (0)	FN	TN

TP: True Positive
FP: False Positive
FN: False Negative
TN: True Negative

Figure 10: Confusion matrix

Moreover, the summarised error classes can be used to calculate numerous classification performance metrics [44–49]. The most commonly mentioned metrics are:

$$Accuracy = \frac{TP+TN}{P+N} \quad (2.13)$$

$$Precision = \frac{TP}{TP+FP} \quad (2.14)$$

$$Recall = \frac{TP}{TP+FN} \quad (2.15)$$

$$F1 - Score = \frac{2 TP}{2 TP + FP + FN} \quad (2.16)$$

Accuracy is the proportion of all correct results out of the total number of cases. The higher the accuracy, the better the trained model. Note that accuracy may not be an adequate measure of performance for imbalanced data sets [50]. In applications where the classes are imbalanced, the classifier can achieve really high accuracy, without representing the basic objective. This means that any data set with an unequal class distribution will represent the minority class much less than the majority classes. This may result in a poor ability of the model to predict these minority classes. The accuracy metric does not take this into account. Moreover, the precision metric shows how precisely the model predicted the positive cases. This is an important metric in some applications. For example, in email spam detection it is crucial to keep the number of false positives as low as possible. A false positive means that a non-spam email (which is actually a negative) has been categorised as spam. The email user would lose important emails, if the model precision is low. On the other hand, the recall metric calculates how many actual positives have been recognised as positives. A false negative means that a spam email (which is actually a positive) has been categorised as non-spam. The email user would receive a lot of spam emails if the model recall is low. A combined metric that includes both precision and recall is called F1-score. The F1-score may be a better choice if the goal is a balance between precision and recall. All these metrics are in the range [0,1].

Accuracy is sensitive to class imbalance, whereas precision, recall and F1-score are asymmetric. Regarding classification errors, the Matthews correlation coefficient (MCC) has often been mentioned in the literature as the best choice [45,48]:

$$MCC = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \quad (2.17)$$

The MCC equation computes the correlation coefficient between the actual class and the predicted class and helps to summarise the information from the confusion matrix into a single value. Unlike the above metrics, the MCC lies in the range [-1,1]. In the case of a perfect classifier (a perfect positive correlation, FN=FP=0), the value of the MCC is 1. In the case of 100 % misclassification (a perfect negative correlation, TP=TN=0), the MCC would get a value of -1. A random classifier has a MCC=0. Furthermore, the MCC is an effective solution to overcome the problem of class imbalance. This is due to the fact that the MCC is perfectly symmetric, includes all values from the confusion matrix and treats all classes with equal importance.

Another useful tool for understanding the core performance of a classifier is called receiver operating characteristics (ROC). The ROC curve is typically plotted in terms of the true positive rate (TPR) and the false positive rate (FPR) [26,46–47]:

$$TPR = \frac{TP}{TP+FN} \quad (2.18)$$

$$FPR = \frac{FP}{FP+TN} \quad (2.19)$$

Where TPR is also known as recall and FPR is closely related to the precision metric (see Equation 2.14). Whereas precision represents what proportion of positive predictions were actually correct, recall defines what proportion of actual positives were correctly identified. Each classifier has some form of threshold or condition that separates the different classes. Moving the threshold in any direction will affect the recall and precision metrics. Interestingly, these two metrics work in opposite ways. Figure 11 illustrates the ROC curve. The x-axis represents the FPR and the y-axis marks the TPR. When both rates are 0, the threshold is such that the model classifies all samples into undesirable classes. If the threshold is ideally moved, the TPR should increase much faster than the FPR (the perfect classifier is illustrated in green). Otherwise the classification is random and unsatisfactory. In the end, the model has classified all samples into the desired class and both rates are 1. The resulting ROC curve finally provides a metric that is independent of the application and represents the fundamental condition of the model. This is the area under the ROC curve (AUC). The higher the AUC, the better the classification. [26]

On the one hand, the ROC curve helps to find the best classification threshold for the given case. On the other hand, the AUC helps to compare different model settings to find the best one.

The choice of the performance metrics also depends on the classification task. Machine learning applications can predict whether it is the actual class (1) or not (0). Another way is to predict a class probability. In the case of a probabilistic classification, the Brier-score metric shows how accurate the probabilities are learned [51]:

$$Brier - Score = \frac{1}{N} \sum_j^R \sum_i^N (f_{ij} - E_{ij})^2 \quad (2.20)$$

Where N is the total number of instances of all classes and R is the number of possible classes. In Addition, f_{ij} represents the predicted probability for class j in the instant i . E_{ij} takes the value 1 if the event occurred in class j or 0 if not. The lower the Brier-score, the better the probabilities are learned.

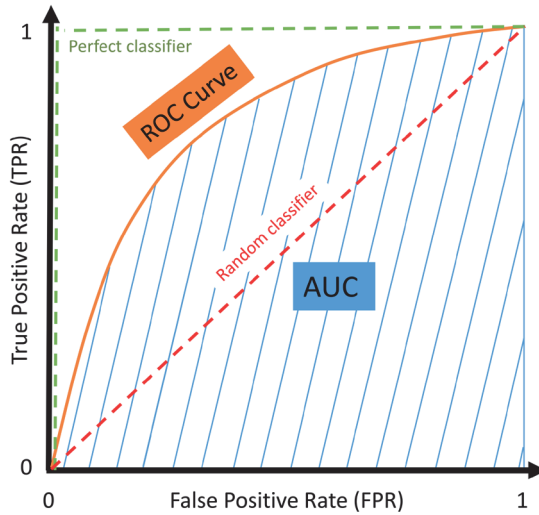


Figure 11: Illustration of the receiver operating characteristics (ROC) curve and the area under the ROC curve (AUC)

2.3.9. Generalisation

Besides the actual learning of a model, which is defined as the ability to adaptively approximate the underlying behaviour from the training data, generalisation is the ability to predict well beyond the training data (Zhang et al. 2000). It seems obvious that generalisation is one of the most important characteristics of a machine learning model. The common use of a classifier is to make good predictions not only on the known and trained data, but also on completely unknown data. It is important to emphasise that generalisation is closely related to the problem of under- or overfitting (Figure 12).

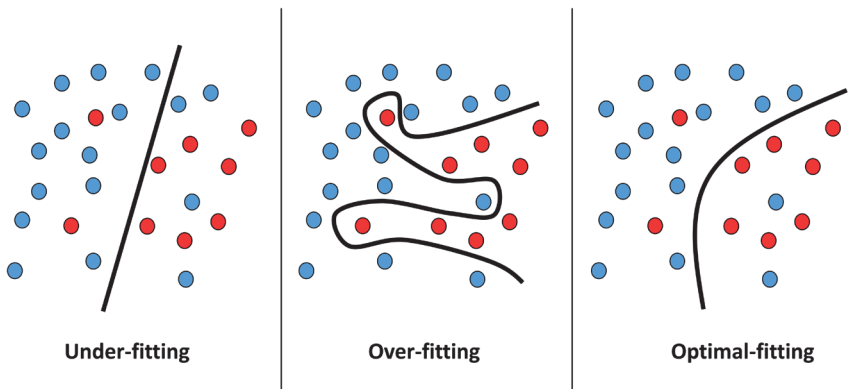


Figure 12: Underfitting, overfitting and optimal fitting in machine learning classification tasks

On the one hand, a powerful data fitting capability of neural networks often leads to the overfitting problem. For example, the neural network has learned perfectly to distinguish the labelled data classes from the given training data set, but has a poor generalisation ability when used for prediction with unknown data. On the other hand, a simple model such as a linear classifier is unlikely to be powerful enough to learn the pattern in the given data set and will tend to underfit. Underfitting and overfitting will affect the generalisation ability of the model. Therefore, the variation of the network size, sample size, model and feature selection should be chosen in such a way that only the underlying pattern in the data set is learned and represented. [52]

A method of determining whether or not the trained model is overfitting is called validation. In the validation process a portion of the training data is split and used to check the generalisation ability by monitoring the performance. The model is

overfitted if the trained model performs poorly on the validation data set. It is important to note that the validation data set is not used to train the model. It is only used to monitor the performance to prevent overfitting. [36]

Another method for improving generalisation is called regularisation. It can be done by modifying the performance function, which is usually chosen to be the mean squared error (MSE). It is possible to improve generalisation by adding a term consisting of the mean of the sum of squares of the network weights and biases [31]:

$$MSE_{Reg} = \gamma \cdot MSE + (1 - \gamma) \cdot MSW \quad (2.21)$$

Where γ is the performance ratio. The mean squared weights and biases (MSW) is defined as follows [31]:

$$MSW = \frac{\sum_{j=1}^n w_j^2}{n} \quad (2.22)$$

Using the performance function results in the network having smaller weights and biases, resulting in a smoother network response without overfitting [31].

2.3.10. Machine Learning Workflow

The last chapters dealt with the basics of supervised learning and neural networks. Finally, the process of building a prediction model based on raw data needs to be illustrated in its entirety. Figure 13 shows an ML workflow using supervised learning (modified from Mandal et al. [53]).

The very first step in developing a supervised machine learning model is to collect the data set. The data set often contains outliers (noise), as well as incorrect or missing data. These data need to be removed or added by data pre-processing. For example, Batista et al. [54] identified the presence of missing data as a relevant data quality issue. The labelled and cleaned data can be divided into a training set and a test set. The training data is used to teach the model, while the test data is used to check how accurate the prediction of the trained model is. In order to obtain a meaningful and non-redundant result, additional pre-processing of the training data is required. Dimensionality reduction, including feature selection and extraction methods, is effective in removing irrelevant and redundant data and increasing the accuracy of the model [55]. A summary of feature selection and fea-

ture extraction techniques is provided by Khalid et al. [55]. This is followed by hyperparameter optimisation (see chapter 2.3.7) and post-processing using appropriate performance metrics (see chapter 2.3.8). After model refinement and final evaluation (using test data), the model can be used to make predictions on new data.

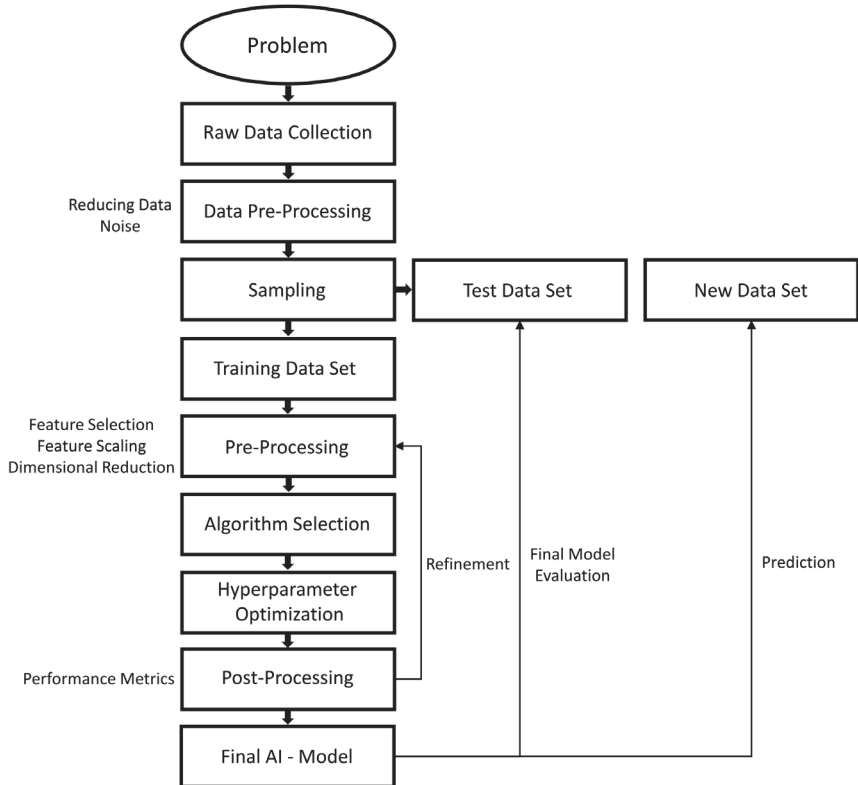


Figure 13: Flowchart for a supervised machine learning model, modified from [53]

3. Objectives and Approach

The aim of this work is to develop a method for predicting process parameters using part quality information, specifically for laser powder bed fusion (PBF-LB/M) and hot isostatic pressing (HIP). Therefore, artificial neural networks have to be trained with as much relevant information as possible. The challenge is to find suitable data that contains enough information about the processes. This involves determining quality characteristics such as internal defects, part density and hardness.

The laser powder bed fusion process using AlSi10Mg is always associated with a large number of internal defects. Pores exist in various types, shapes and sizes and they have a process-related origin. Therefore, pores can be considered as a process fingerprint that contains all relevant information about process parameters and final quality. Moreover, the HIP parameters are the main determinant of the pore closure result during the treatment. Hence, it should be possible to find enough information in the change of pores while varying the process parameters and build an ML prediction model from these data. Because of the idea of using pores as a source of information, computed tomography seems to be the best choice to collect the data. Many previous investigations have focused on defect detection using X-ray data and presented accurate evaluations of pore distributions in additively manufactured parts [56–59].

Furthermore, supervised machine learning seems promising for classification tasks. Hence, the approach is to train a neural network with labelled pore data from X-ray scans. Figure 14 and Figure 15 show the general approach of this work to achieve the goal of parameter prediction using pores as the corresponding quality information. Besides the pore data, hardness and part density measurements will provide additional quality information for the regression neural networks. In order to train a supervised learning algorithm, the input and output data must be known. On the one hand, AM parameter information about the hatch distance, layer thickness and scanning speed must be available. In order to describe the HIP process, information on treatment time, pressure and temperature is required. On the other hand, the corresponding porosity, hardness or part density information is needed as well. Therefore, many specimens containing this information need to be produced and tested. In addition to the actual data generation, the data needs to be processed in an appropriate manner. A reliable method of pore classification is required, as well as extensive checks on the accuracy and validity of the data. Data quality is one of the most important aspects in the development of

a successful ML model. If the data does not represent the physical reality, the learned model will not predict the reality as well. Therefore, data preparation and evaluation play an important role and will be developed and analysed in this work. Furthermore, the ML model will be built, evaluated and validated.

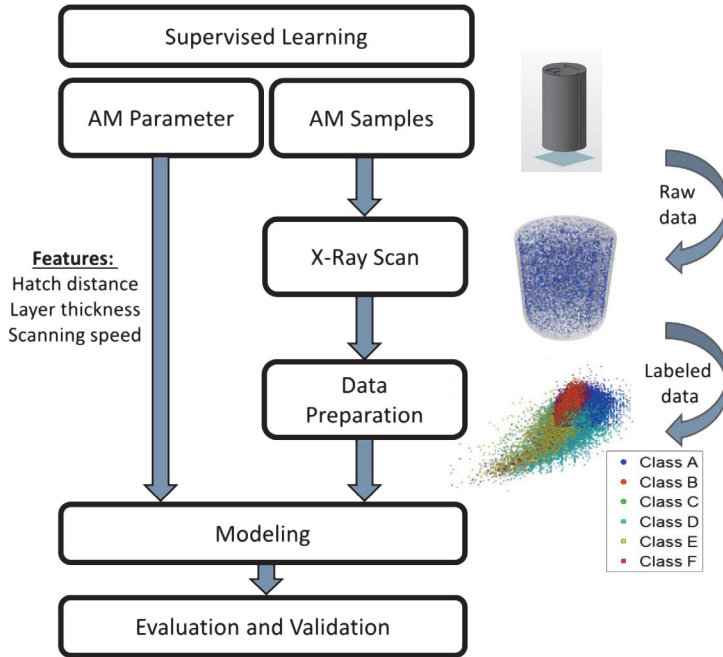


Figure 14: Supervised learning approach for pore-based AM parameter prediction

After presenting the basics of laser powder bed fusion, hot isostatic pressing and supervised machine learning in the previous chapter, the following chapter describes the used methods. Particular attention will be paid to the used AM and HIP machines, as well as to the chosen parameter settings and specimen designs. Moreover, the used measurement equipment (e.g. computed tomography) as well as the used approach for the construction of the neural networks, including the model architectures and settings will be presented.

It is important to note that this work is a publication-based research. For this reason, the results are divided into two chapters. The first chapter deals with the data preparation and evaluation, which is entirely executed in peer-reviewed publications. The second chapter focuses on the predictions of the ANN model. All 3 peer-reviewed publications are presented after the methods chapter, followed directly by the presentation of the neural network results. These findings will form the basis for the further discussion and interpretation. The final review will summarise the results and give an outlook on further research topics.

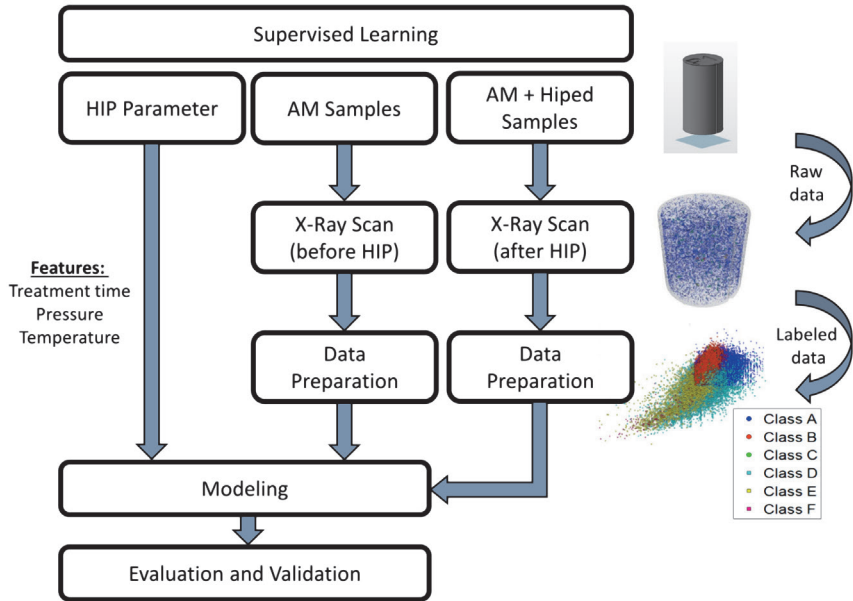


Figure 15: Supervised learning approach for pore-based HIP parameter prediction

4. Methods

4.1. PBF-LB/M and HIP Process

The analysed cylindrical specimens were manufactured at FIT AG using a SLM500 PBF-LB/M machine (SLM Solutions, Lübeck, Germany). The SLM500 is equipped with a Nd:YAG laser ($\lambda = 1064 \text{ nm}$) with a maximum laser output of 400 W. The working point of the laser is usually at 350 W. The building direction was chosen to be vertical to the building platform. All specimens were built using AlSi10Mg powder (Tekna Advanced Materials Inc., Sherbrooke, Canada). The chemical composition of the used powder can be seen exemplarily in Nudelis et al. [17]. An overview of the PBF-LB/M process parameters for the manufactured specimens are listed in Table 2 and Table 3. A total of 32 PBF-LB/M parameter sets were tested and evaluated. Scanning speed, hatch distance and layer thickness were varied. Finally, 3,066,249 pores from 96 cylindrical specimens formed the pore database for the PBF-LB/M networks. Each parameter set is represented by 3 specimens.

Part density can also be predicted using a neural network. Therefore, the part density of 96 specimens were measured by means of the Archimedes principle. The specimens are the same as those used for the pore type prediction. Moreover, the database was further extended using the Archimedes measurement tolerance ($\pm 0.07 \%$) calculated from the standard deviations of all 3 specimens over all 32 parameter sets. Generally speaking, the part density measurements can have a spread of $\pm 0.07 \%$. This spread was used to generate more data for the network training. All measurements were offset by [$\pm 0.01 \%$; $\pm 0.02 \%$; $\pm 0.03 \%$; $\pm 0.04 \%$], which is still clearly within the measurement tolerances. This generates additional 768 part densities. A total of 864 density values were used to train the neural network.

Parameter Set	Scanning Speed (mm/s)	Hatch Distance (mm)	Layer Thickness (μm)	VED (J/mm^3)
1	1000	0.15	40	58.33
2	1000	0.2	40	43.75
3	1250	0.15	40	46.67
4	1250	0.2	40	35.00
5	1500	0.15	40	38.89
6	1500	0.2	40	29.17
7	1750	0.15	40	33.33
8	1750	0.2	40	25.00
9	1000	0.15	80	29.17
10	1000	0.2	80	21.87
11	1250	0.15	80	23.33
12	1250	0.2	80	17.50
13	1500	0.15	80	19.44
14	1500	0.2	80	14.58
15	1750	0.15	80	16.67
16	1750	0.2	80	12.50

Table 2: PBF-LB/M parameter sets 1–16 for ML training as well as the calculated volumetric energy densities (VED)

The melting process can be described by the induced volumetric energy density (VED) in the deposited metallic powder. The definition of the classical and modified versions of VED is described in chapter 2.1. The classical definition of VED uses the ratio between the laser power P_L (W) and the product of the layer thickness t (mm), the laser scanning speed v (mm/s) and the hatch distance h (mm). The modified version of the VED also requires the material properties (absorption factor β and thermal diffusivity α) as well as the influence of the spot size diameter ϕ . The layer thickness is not included in the modified version of the VED. The pore analyses in publication II (Nudelis et al. [17]) showed that the pore formation can be well described using the modified volumetric energy density (VED). The analy-

sis results are easier to describe using only one variable that includes all parameter information. In this work, the classical definition of the VED was used. This is due to the fact that the spot size diameter is a constant value of 0.08 mm and the layer thickness is varied in all parameter settings (ML training). The classical VED includes all varied parameters and will help to interpret the prediction and measurements results. All VED values are listed in the Table 2, Table 3 and Table 4.

Parameter Set	Scanning Speed (mm/s)	Hatch Distance (mm)	Layer Thickness (μm)	VED (J/mm^3)
17	1000	0.125	30	93.33
18	1000	0.175	30	66.67
19	1250	0.125	30	74.67
20	1250	0.175	30	53.33
21	1500	0.125	30	62.22
22	1500	0.175	30	44.44
23	1750	0.125	30	53.33
24	1750	0.175	30	38.09
25	1000	0.125	60	46.67
26	1000	0.175	60	33.33
27	1250	0.125	60	37.33
28	1250	0.175	60	26.67
29	1500	0.125	60	31.11
30	1500	0.175	60	22.22
31	1750	0.125	60	26.67
32	1750	0.175	60	19.05

Table 3: PBF-LB/M parameter sets 17–32 for ML training as well as the calculated volumetric energy densities (VED)

In order to check the generalisation ability of the PBF-LB/M network beyond the known 32 parameter sets, an additional test with 5 completely new parameter sets is carried out. This additional test represents 13.5 % of the total parameter data

and is expected to adequately capture potential variety. The additional PBF-LB/M parameter sets are listed in Table 4.

Parameter Set	Scanning Speed (mm/s)	Hatch Distance (mm)	Layer Thickness (μm)	VED (J/mm^3)
1	1125	0.1275	35	69.72
2	1600	0.17	35	36.76
3	1400	0.155	70	23.04
4	1200	0.12	70	34.72
5	1700	0.19	70	15.48

Table 4: PBF-LB/M parameter sets for additional generalisation check as well as the calculated volumetric energy densities (VED)

The used HIP parameters are listed in Table 5. The samples were treated at temperatures of 480 °C or 540 °C, pressures of 300 bar or 2,000 bar, as well as dwell times of 30 min or 90 min. All cylindrical specimens were produced with a laser power of 350 W, a laser scanning speed of 1,150 mm/s, a layer thickness of 50 μm and a hatch spacing of 0.17 mm. The spot size diameter of the laser beam was set to 0.08 mm. The cylindrical specimens were then HIPed at FIT AG using a Quintus 32 1400M URQ (Västerås, Sweden). The furnace was filled with argon gas. A total of 1,489,857 pores from 48 cylindrical specimens before and after HIP formed the pore database. Each parameter set is represented by 6 specimens.

In addition to the pores, the hardness was also determined in order to train a neural network. Therefore, a total of 28 samples from 8 parameter variations (3 specimens each parameter set, Table 5) as well as reference samples (4 specimens) without any HIP treatment were analysed. The samples are the same as for the HIP pore type prediction. But, only 3 out of 6 samples were used for the hardness measurement (a total of 3 indentations per sample). Besides that, the database was further extended using the calculated hardness measurement tolerance (± 0.45 HBW), which was determined by the standard deviations of all 3 specimens and their 3 indentations over all 8 parameter sets (72 measurements). The hardness has a spread of ± 0.45 HBW. This spread was used to generate more data for the network training. All measurements were offset by [± 0.1 HBW; ± 0.2 HBW; ± 0.3 HBW; ± 0.4 HBW]; which is still clearly within the measurement tolerances. This provides additional 672 hardness values. In total, 756 hardness values are available for training the neural network.

Parameter Set	Time (min)	Pressure (bar)	Temperature (°C)
1	30	300	540
2	30	300	480
3	30	2000	480
4	90	300	540
5	90	300	480
6	30	2000	540
7	90	2000	480
8	90	2000	540

Table 5: HIP parameter sets for ML training

To check the generalisation ability of the HIP network beyond the known 8 parameter sets, an additional test with 3 unknown parameter sets is mandatory. The additional HIP parameter sets are listed in Table 6. Besides the process parameters (time, pressure and temperature), the initial pore distribution prior to HIP plays an important role. All predictions are based on the mean initial pore distribution, calculated over all measured HIP samples (40.69 % (class A), 9.14 % (class B), 0.02 % (class C), 36.31 % (class D), 13.34 % (class E), 0.49 % (class F)).

Parameter Set	Time (min)	Pressure (bar)	Temperature (°C)
1	40	400	500
2	35	200	485
3	15	1000	490

Table 6: HIP parameter sets for an additional generalisation check

4.2. Specimen Design and Measurement Equipment

4.2.1. Computed Tomography

A simple cylindrical specimen shape (10 mm in diameter, 18 mm in height) was chosen for the X-ray scans. The reason for this is the symmetrical geometry, which allows the part to be scanned with the same radiated wall thickness, thus reducing CT artefacts. X-ray scans were made using a Diondo d2 microfocus CT system (Hattingen, Germany) with a minimum voxel size of $9.659 \mu\text{m}^3$. The specimen was scanned in 1500 projections with 360° sample rotation (1.4 s integration time per projection) using a power output of 9.5 W and a voltage of 190 kV. Reconstruction of the raw CT data into a 3D model was performed using VGSTUDIO MAX 3.1.0 64 (Volume graphics, Heidelberg, Germany). The VGDefx algorithm was used for porosity analysis. The analysed region of interest (ROI) had a volume of 785.4 mm^3 .

4.2.2. Archimedes Principle

For the Archimedes density measurements the same cylindrical specimens were used (described in chapter 4.2.1). To determine the density of a cylinder, it is weighed once in air and then in a liquid of known density. The formula in Equation 4.1 describes the calculation of the part density [60].

$$\rho_{part} = \frac{m_{air}}{m_{air} - m_{liquid}} \cdot \rho_{liquid} \quad (4.1)$$

Where $\rho_{part} \left(\frac{\text{g}}{\text{cm}^3}\right)$ is the density of the part, $m_{air} \text{ (g)}$ is the measured mass in air and $m_{liquid} \text{ (g)}$ is the measured mass in the liquid (typically ethanol). Moreover, $\rho_{liquid} \left(\frac{\text{g}}{\text{cm}^3}\right)$ represents the density of the liquid. Measurements were made using a Kern & Sohn AET 200-4 NM hydrostatic balance (Balingen-Frommern, Germany). The accuracy of the measurements is 0.1 mg.

4.2.3. Hardness Measurement

Hardness measurements (according to Brinell EN ISO 6506) were carried out on the same cylindrical specimens (described in chapter 4.2.1) using a Mitutoyo HR-522 Wizard (Neuss, Germany). Unlike CT and Archimedes, hardness measurement is a destructive test method. The Brinell hardness test determines the hardness by pressing a hardened ball (typically steel or carbide) into the surface of the material with a known force. The diameter of the indentation (left by the ball) is

measured. These values are needed to calculate the Brinell hardness according to EN ISO 6506 (Equation 4.2).

$$HBW = 0.102 \cdot \frac{2F}{\pi D^2 (1 - \sqrt{1 - d^2/D^2})} \quad (4.2)$$

Where F (N) is the load, D (mm) represents the diameter of the indenter and d (mm) defines the mean diameter of the indentations. In this work, the indenter has a diameter of $D=2.5$ mm, penetrating the material with a force of $F = 612.9$ N. The mean diameter of the indent was determined by measuring the horizontal and vertical diameters of the indentation.

4.3. ML Model Settings

The neural network approach was chosen to provide reliable process parameter or pore class prediction using machine learning. Figure 16, Figure 17 and Figure 18 show the used neural network architecture for the AM and HIP application. All classification based neural networks, including the pore data, deal with a multi-class classification problem for predicting pore types. All neurons within the hidden layers are connected with the log-sigmoid transfer function. This prevents negative outputs, which are simply not present in this kind of classification and regression problems. The log-sigmoid transfer function normalises the input (any value between plus and minus infinity) to a finite range of positive values (0 to 1). Furthermore, the log-sig function is differentiable, which is necessary in multi-layer back-propagation networks (see chapter 2.3.4). The output layer uses a softmax transfer function to produce the classification outcome (see chapter 2.3.3).

The number of hidden layers is limited to 5. Each hidden layer may contain up to 20 neurons. The choice of the optimal number of layers and neurons is determined by hyperparameter optimisation methods. The theory is described in chapter 2.3.7. All parameters based on properties related to data characteristics or the capacity of the learning algorithm are called hyperparameters. Hyperparameters must be set manually before the training starts.

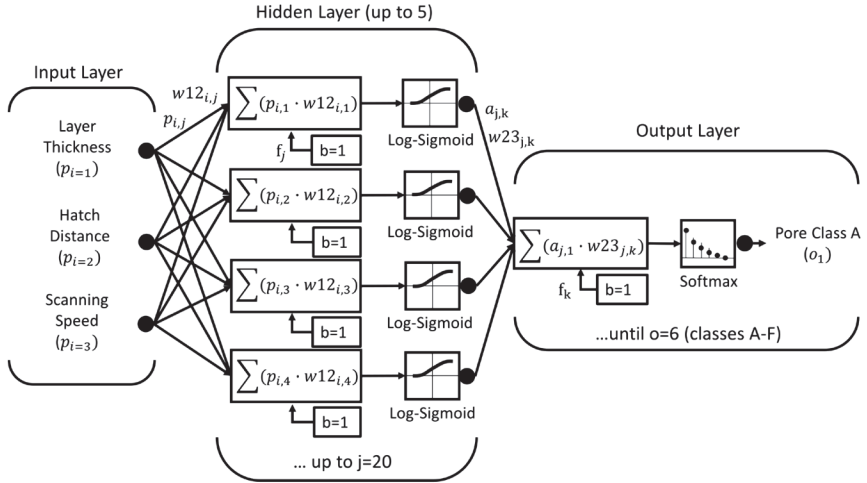


Figure 16: Artificial neural network for AM process parameter/ pore class prediction

In the context of this work, the following hyperparameters are relevant:

- Normalisation
- Number of hidden layers
- Number of neurons at each layer
- Transfer and performance (loss) function
- Initialisation and training function

The neural network for the AM process parameters/ pore class prediction takes as input the layer thickness (μm), the hatch distance (mm) and the scanning speed (mm/s). The output consists of the resulting pore classes A–F (categorised according to the classification method in Nudelis et al. [16]).

The neural network for the HIP process parameters/ pore class prediction takes as input the treatment time (min), the pressure (bar), the temperature ($^{\circ}\text{C}$), as well as all six pore classes (that existed in the part before HIP) and as output the hipped pore classes. All pores are also categorised according to the classification method in publication I (Nudelis et al. [16]). All continuous input and output values are normalised to standard values using the mapstd function. Mapstd processes the data by transforming the mean to 0 and the standard deviation to 1. The classified inputs and outputs (all pore types) are already available in a binary structure, so an additional normalisation is not needed.

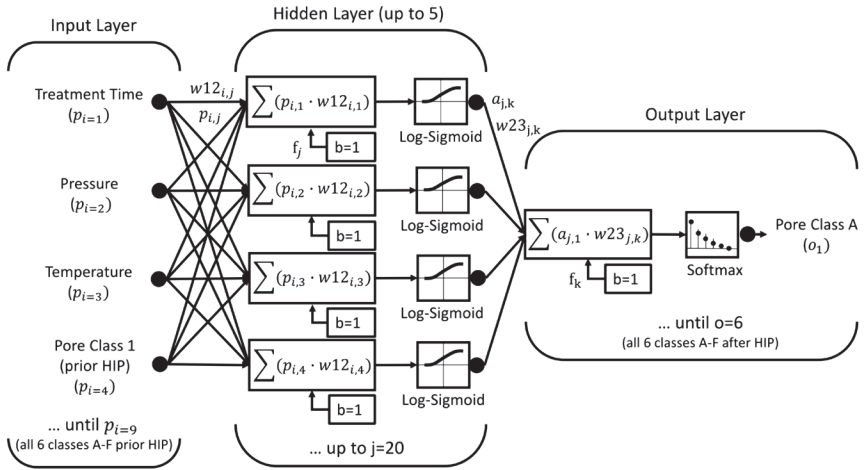


Figure 17: Artificial neural network for HIP process parameter/ pore class prediction

The optimal number of layers, as well as the number of neurons in each layer, is analysed using the grid search approach (see chapter 2.3.7). This describes the safest way to find the best set of hyperparameters by training the data set on every relevant combination. Due to a manageable number of hyperparameter variations and still acceptable training times, grid search is the better choice compared to random search. The number of layers is analysed in single steps from 1 up to 5 layers (deep neural networks). Moreover, the number of neurons is varied from 1 single neuron up to 20 neurons per layer. First, a narrow neural network consisting of 1–10 neurons (per layer) is trained. In a second training phase, wide neural networks with 12–20 neurons (per layer) will be analysed.

Matlab R2021b (Natick, MA, USA) was used to create and train all neural networks. The transfer, performance, training and initialisation functions are set as constant hyperparameters in all neural network variants. The hidden layer uses a

log-sigmoid transfer function and the output layer uses the softmax transfer function to generate the classification outcome. In the case of a regression outcome, a purelin transfer function is used in the output layer. When it comes to choosing a loss function (also called performance function), the cross-entropy and mean squared error (MSE) are the main types to use when training a neural network model. Cross-entropy is used for classification problems, while MSE calculates the errors for networks with continuous output values. Scaled conjugate gradient back-propagation training (trainscg) was used as the training function. The trainscg function updates weights and biases according to the scaled conjugate gradient method. Trainscg can be used for any network as long as its weights, inputs and transfer functions are derivable functions. More information on the trainscg algorithm can be found in [61].

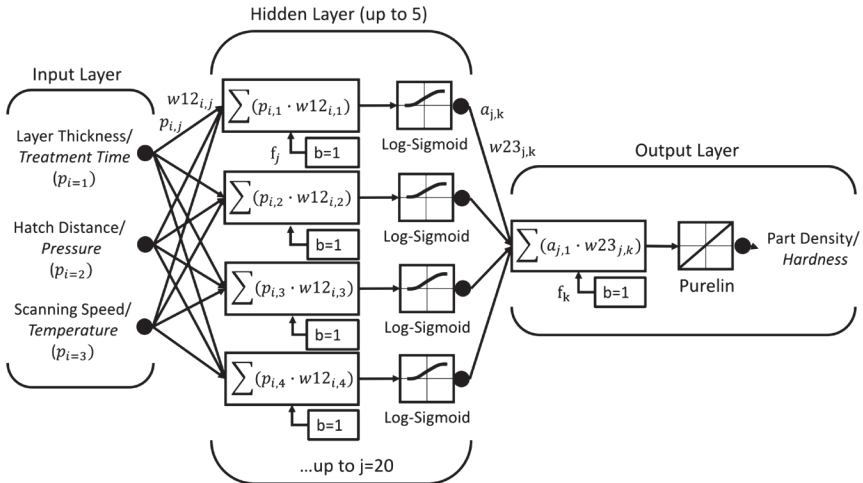


Figure 18: Artificial neural network for AM/ HIP process parameter/ part density and hardness prediction

All networks are trained on the training data (70 % of all data) until the performance on the validation data (15 %) begins to decline, indicating that generalisation has peaked. The test data (15 %) provides a completely independent test of network generalisation. The data were randomised before being split into training, validation and test data sets. Due to the lack of data variation, an additional generalisation check on new data (unknown parameter variations) is necessary as well as explained in more detail below.

The training will stop if any of these conditions occur:

- The maximum number of epochs is reached
 - For classification problems: 1000 epochs
 - For regression problems: 10000 epochs
- Performance (loss) gradient falls below the minimum gradient goal
 - Minimum Gradient = 10^{-6}
- Validation performance has increased more than 6 (for classification problems)/ 10 (for regression problems) times since it decreased

Before training can begin, all initial weights and biases must be set. The Nguyen-Widrow layer initialisation function (initnw) was used to initialise the weights and biases of the layer. This algorithm distributes the active region of each neuron in the layer over the input space of the layer to select the initial values. The values contain a degree of randomness, so they are not the same each time the initnw-function is used. The function is based on Nguyen et al. [62].

In terms of general neural network architecture, two different approaches have been tried. On the one hand, a classic fully connected network, where all layers and their neurons are connected to each other. All regression and classification tasks used the fully connected network. On the other hand, a separated network, where there are several neural lines for each output variable. Each neural line contains its own hidden layer. The neurons of each hidden layer are fully connected to the next hidden layer, but only within the neural line. The hidden layer and its neurons are not connected to the hidden layers and neurons of any other neural line. Only the output layer (softmax transfer function) connects the neural lines to a merged outcome. This model architecture was implemented for the classification tasks where multiple pore types need to be predicted. The presence of an unequal class distribution could result in the minority class being represented to a much lower extent than the majority classes. This problem is called class imbalance and deals with a disproportion of class examples. The used separated neural network design is inspired by the class binarisation techniques OVO (one-vs-one) and OVA (one-vs-all) (see chapter 2.3.6), which can be very useful in overcoming the problem of imbalanced data. Both types of model architectures are shown schematically in Figure 19.

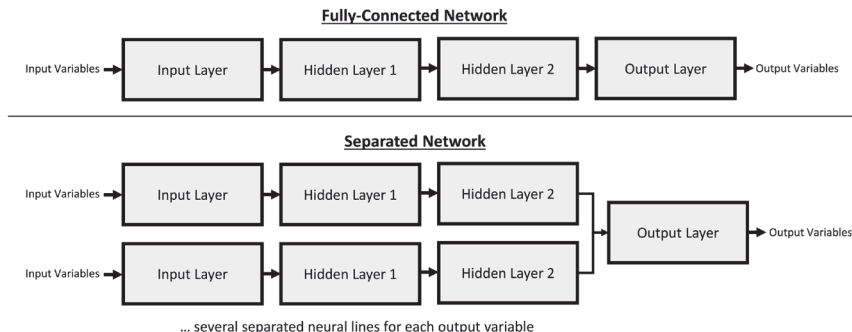


Figure 19: Illustration of the difference between fully connected and separated networks

Finally, performance metrics are used to evaluate the neural network variants from the grid search process. The used performance metrics (suitable for classification problems) are the Brier-score, the area under the ROC curve (AUC), as well as the cross-entropy. Metrics calculated from the confusion matrix (accuracy, precision, recall, F1-score and the Matthews correlation coefficient (MCC)) were not used. Accuracy is not an adequate measure of performance due to the imbalanced data set [50]. For instance, the MCC provides more reliable information and treats all classes with equal importance [45,48]. However, Brier-score, AUC and cross-entropy provide sufficient information for model evaluation and make the use of other performance metrics unnecessary. Performance metrics for regression problems are the mean square error (MSE) and the coefficient of determination (CoD) also called R^2 (R-squared). Each metric provides its own information about the model performance and highlights the problems (type of error). More information about each of these performance metrics can be found in chapter 2.3.8.

Nevertheless, the generalisation ability of the model can be quite limited due to the lack of data variations (see chapter 2.3.9) and a small database (mostly in the case of the regression tasks). The previously mentioned performance metrics only have the ability to represent the known data variations. In order to check the ability of the network to predict unknown data variations, an additional generalisation check is performed. The complete ML workflow including the most relevant settings is illustrated in Figure 21.

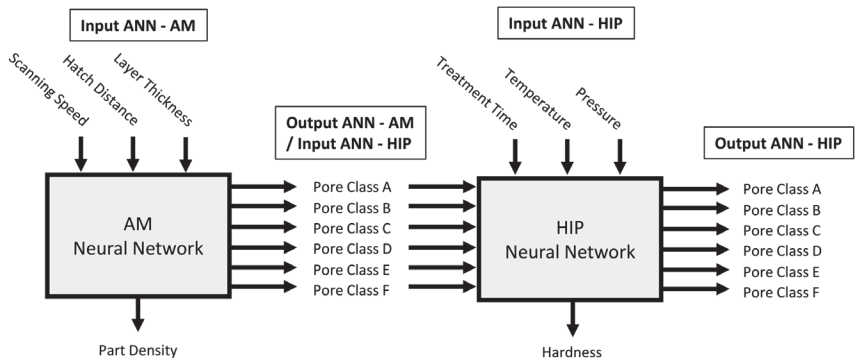


Figure 20: Combined approach of ML prediction of AM and HIP process parameters/ pore distributions, as well as part density and hardness

An overview of all input and output values of the AM and HIP networks is shown in Figure 20. The AM network is able to predict part density and pore classes A–F after the manufacturing process using defined process parameters for the scanning speed, hatch distance and layer thickness. The HIP network predicts the hardness of the parts and the leftover pores after the HIP treatment using the information on the pre-existing pore classes A–F after the manufacturing process as well as the treatment time, temperature and pressure during the HIP cycle. Both networks are trained separately with their own database and data variations. The aim of this work is to create networks that can be used separately or in combination. For example, the predicted pore classes A–F from the AM network can be used as input values for the HIP network.

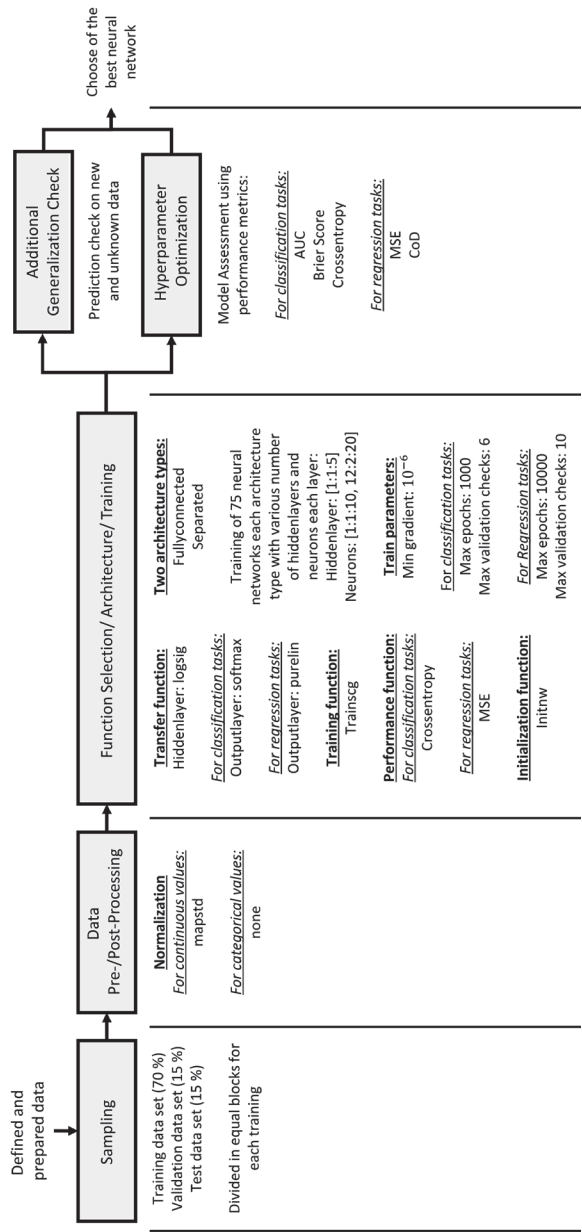


Figure 21: ML workflow including the most relevant settings

5. Publication I: A Novel Classification Method for Pores in Laser Powder Bed Fusion (Nudelis et al. [16])

5.1. Abstract

Pores can be seen as an individual process fingerprint. This is due to the fact that the formation of pores is highly dependent on the applied PBF-LB/M process parameters. It seems to be obvious that pores can perfectly serve as a data source for supervised machine learning applications. The aim of the first publication was to qualify a new approach to pore classification using X-ray tomography. The main advantage of X-ray scans is the possibility to collect a considerable amount of 3-dimensional pore information. This data provides relevant information on the position, shape, size, volume fraction and number of pores, allowing pores to be classified into different pore classes. Several investigations have been carried out to improve the understanding of pores and their impact on quality standards. Firstly, the influence of pore size, shape, and location on crack initiation in AISi10Mg parts produced by PBF-LB/M was investigated. For this purpose, 26 selected pores of different morphology (out of a total number of 39228 detected pores) were analysed by means of finite element analysis (FEA). Furthermore, the correlations between the pore characteristics and the degree of stress concentration were analysed using fracture mechanics determinations. The result is an evaluated novel pore classification method that helps to collect the necessary labelled data for supervised learning application (e.g. neural networks).

The developed classification method classifies pores according to their size (small, medium, large) and their shape (spherical or irregular-shaped). Three shape indicators (compactness, sphericity and BB-factor), as well as the diameter as a size indicator are required for an accurate pore classification. Optionally, a classification by location (internal pores or near-surface pores) can be made.

5.2. Summary of Key Findings

- All three shape indicators (compactness, sphericity and BB-factor) must be used to define the 3-dimensional pore shape as accurately as possible in the irregular and spherical classes. Generally speaking, the combined use of sphericity, compactness and bounding box factor will lead in a significant reduction in pore shape misclassification.
- Stress concentrations at pores are highly dependent on the pore shape and loading direction. The FEA results show that the exact value of sphericity and compactness cannot be used as a predictor of high stress concentrations. On the one hand, irregularly shaped pores show a completely different result in stress concentration under different load directions. On the other hand, spherical pores are independent of load direction.
- The highest pore stress concentrations occurred in pores with a large cross-sectional transition. Nevertheless, knowledge of the exact pore geometry is irrelevant unless the loading direction is also known.
- In particular, large, near-surface and irregularly shaped pores will dictate the occurrence of critical failure of the component. These pore classes should be reduced by using adapted process parameters or suitable post-processing methods such as hot isostatic pressing.
- The developed classification method using X-ray data can be used to provide a considerable amount of labelled pore data for supervised learning applications (e.g. neural networks).

The contribution of the author to publication I is summarised in Table 7.

	Conceptualisation	Elaboration of contents	Writing – review and editing	Total
N. Nudelis	95 %	100 %	90 %	95 %

Table 7: Percentage of the author's contribution to publication I

6. Publication II: Defect-based Analysis of the Laser Powder Bed Fusion Process using X-Ray Data (Nudelis et al. [17])

6.1. Abstract

Internal defects are the inevitable byproduct of the current state of laser powder bed fusion (PBF-LB/M) of Al alloys. However, pores can be seen as an individual process fingerprint that contains a lot of information about the process conditions. In order to exploit this individual information, process-induced pores need to be analysed at a higher level of detail. The aim of the second publication was to clarify the correlation between pores and PBF-LB/M process parameters in AlSi10Mg components. Therefore, the novel classification method from publication I was used to classify a total number of 2,939,830 pores detected in 96 cylinders. The mechanisms of pore formation were changed by varying the volume energy density (VED), e.g. by using different laser scanning speeds. Additionally, the effect of powder preparation scan strategies on the pore formation was analysed in the pre-heating and pre-sintering study. These two scanning strategies were used to prepare the powder in situ prior to the actual melting process. Finally, the general reproducibility as well as the influence of different lasers and shielding gas flows were investigated.

6.2. Summary of Key Findings

- In general, the higher the introduced energy into the powder bed (VED), the fewer irregularly shaped pores (most likely lack-of-fusion pores) and the more spherical-shaped pores (most likely hydrogen and keyhole pores) occurred.
- The use of prior powder preparation scan strategies (such as pre-sintering or pre-heating) reduces the total number of pores by up to 45 % at high scanning speeds.

- As the scanning speed is increased, the number of spherical pores tends to decrease and more irregularly shaped and larger pores appear. By using the pre-heating process at a scanning speed of 1000 mm/s, the formation of spherical pores was drastically reduced.
- Condensate and vapour plume from the melting process could contaminate the laser's protective window, leading to the formation of irregularly shaped pores (lack-of-fusion). Besides that, the shielding gas flow seems to stimulate the formation of lack-of-fusion pores (especially pore class D) on the gas outlet side, probably caused by weld spatter.
- The use of X-ray data in combination with the novel pore classification method (from publication I) proves to be a suitable tool to determine the quality of AISi10Mg components based on process parameters and conditions.

The contribution of the author to publication II is summarised in Table 8.

	Conceptualisation	Elaboration of contents	Writing – review and editing	Total
N. Nudelis	95 %	100 %	90 %	95 %

Table 8: Percentage of the author's contribution to publication II

7. Publication III: Pore Tracing in Additive Manufactured and Hot Isostatic Pressed Components (Nudelis et al. [18])

7.1. Abstract

Hot isostatic pressing (HIP) is a densification process involving the simultaneous application of an elevated temperature and a high gas pressure acting uniformly in all directions. The use of HIP on additively manufactured components is recognised for its ability to produce high density parts with microstructurally homogeneous properties. However, the knowledge of the exact pore closing behaviour is not yet fully explored. For this reason, publication III focuses on laser powder bed fused (PBF-LB/M) and hot isostatic pressed (HIP) AlSi10Mg components and process-related pores that occur. The publication explores the effect of HIP on various pore characteristics such as pore shape, size and type. In order to retrieve the pores before and after HIP, a pore tracing method based on the k-nearest neighbours approach was developed. The method evaluates X-ray data before and after HIP, which allows the remaining pores to be matched with the initial pores. In this work, a total of 274,886 pores from eight different HIP settings were classified, matched, examined and discussed. The novel classification method from publication I was used to classify the detected pores into appropriate classes. By using the novel pore tracing method in combination with the classification method from publication I, it is possible to observe the pore closing behaviour for different HIP settings. Furthermore, the exact transformations can be tracked, providing a comprehensive insight into the change of pore characteristics during HIP.

7.2. Summary of Key Findings

- Irrespective of the HIP parameter setting and the initial pore size and shape, all pores started to transform their shape towards irregular shapes and small pore diameters. Increasing pressure, time and temperature only accelerated the pore transformation.
- The finding clearly demonstrate that larger pores close faster than smaller ones. Spherical pores also took longer to close than irregularly shaped pores.

- The use of longer treatment time, as well as higher pressure and temperature settings leads to a more successful densification result.
- The presented pore tracing method can be used to analyse the effect of hot isostatic pressing on the pore closing behaviour and thus serve as a data source for supervised learning methods such as neural networks.

The contribution of the author to publication III is summarised in Table 9.

	Conceptualisation	Elaboration of contents	Writing – review and editing	Total
N. Nudelis	95 %	100 %	90 %	95 %

Table 9: Percentage of the author's contribution to publication III

8. Machine Learning

The aim of this chapter is to develop suitable artificial neural networks for the prediction of PBF-LB/M and HIP process parameters based on their quality characteristics such as pore types, part density and hardness. The development approach for all neural networks is described in chapter 4.3. Detailed information on the sample fabrication and measurement process is given in chapter 4.1 and 4.2. Hyperparameter optimisation, model selection and evaluation as well as the discussion of the prediction results are presented in this chapter.

All machine learning models require a metric to judge their performance. The area under the ROC curve (AUC), the Brier-score as well as the cross-entropy were chosen to evaluate the trained classification models. The AUC and Brier-score were also calculated separately for each pore type. The coefficient of determination (CoD) and the mean squared error (MSE) were used to evaluate the trained regression models. The hyperparameter optimisation includes the analysis of different networks with different number of hidden layers (1–5) and different numbers of neurons per hidden layer (1–20). The results of the hyperparameter optimisation are illustrated in colour maps.

8.1. Hyperparameter Optimisation and Model Choice (PBF-LB/M)

8.1.1. Fully Connected ANN Model for Pore Types

Finally, 3,066,249 pores from 96 cylindrical specimens formed the pore database for training the following PBF-LB/M neural networks. All 32 process parameters are listed in Table 2 and Table 3. Moreover, the pores were classified according to the classification method described in publication I (Nudelis et al. [16]).

8.1.1.1. Performance Metrics – AUC, Brier-Score, Cross-Entropy

Figure 22 shows the AUC colour maps for each pore type A–F for all 75 fully connected network variants. The definition of the ROC-curve and the resulting AUC metric are summarised in chapter 2.3.8. However, the AUC metric is independent of the application and represents the fundamental condition of the model. The higher the AUC, the better the classification. The AUC performance metric helps to compare different model settings to find the best one. An AUC value of 1 de-

scribes a perfect classifier, while a value of $AUC = 0.5$ indicates a random classifier. An $AUC = 0$ means that no classification was correctly predicted. In general, the fully connected networks have AUC values between 0.42–0.86. The calculations show that the AUC values differ from one pore type to another. It is important to emphasize that the pore types are collected in an imbalanced data set. All classified pores from all 32 parameter sets are summarised in the Appendix A.2. As can be seen there, the small pore types A and D appear in larger numbers than the larger pore classes B, C, E, F. Pore class C is the rarest pore class. The minority class C demonstrates the strongest dependence on the number of hidden layers and their neurons. For all pore classes, more neurons per hidden layer lead to better AUC values and thus to better predictions. There is no clear dependence of the AUC on the number of hidden layers.

In the case of a probabilistic classification, the Brier-score metric (Equation 2.20) shows how accurately the probabilities are learned. Before the Brier-scores can be analysed, the meaning of the calculations needs to be clarified. The Brier-score metric was calculated based on the independent test data set (15 %). The Brier-score checks this way the generalisation ability of the network based on this test data set. Generalisation means how accurately the model predicts outputs with unknown inputs. Note that no data was removed from the original data set during the data pre-processing. All pores in the imbalanced data set were used. This is because the output describes a pore distribution (probability). Any manipulation of the original data set (pore classes) could affect the distribution. Only 32 parameter sets are included in the data. Most likely the test data set is not variable enough compared to the training and validation data set to check the generalisation ability beyond the 32 parameter variations. Figure 23 illustrates the cross-entropy of the training (70 %), validation (15 %) and test (15 %) data sets for all 75 neural network variants. It can be seen that the cross-entropy for the training, validation and test data sets are very similar.

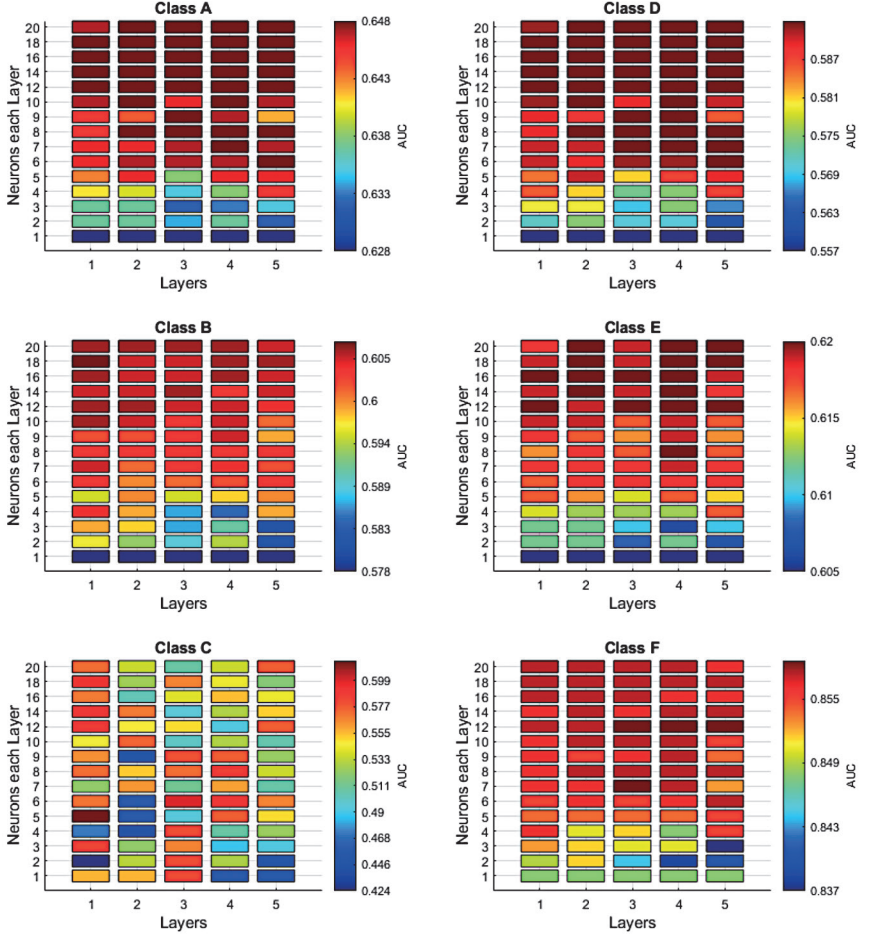


Figure 22: AUC for pore classes A–F in different fully connected neural networks (for PBF-LB/M prediction) with different numbers of hidden layers and neurons in each hidden layer

This indicates that the training, validation and test data sets consist of very similar data. Hence, the shown Brier-score only checks how accurately the network predicts the known 32 parameter sets with new but similar data information. The generalisation check beyond these known 32 parameter sets is performed with an additional test data set using complete unseen parameters.

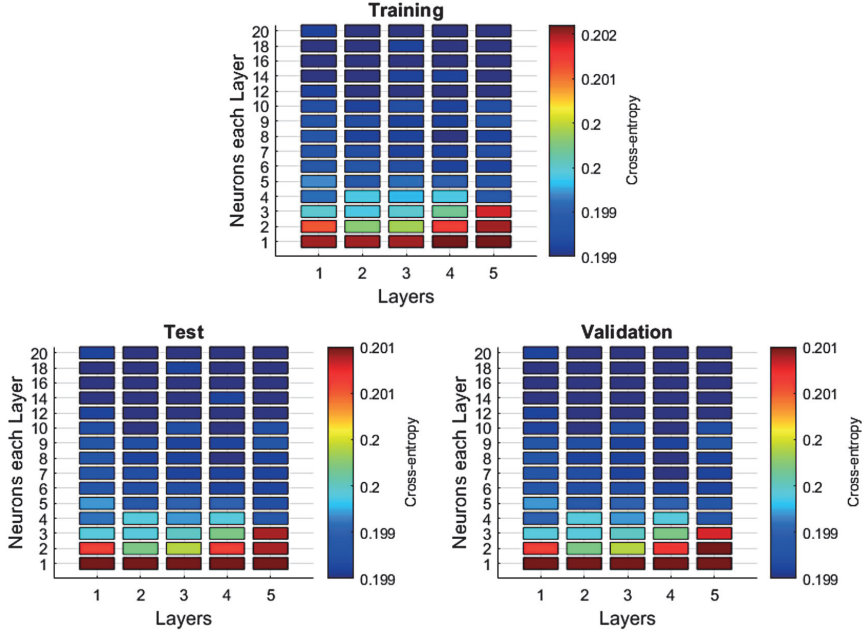


Figure 23: Cross-entropy for the training, test and validation data set in different fully connected neural networks (for PBF-LB/M pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

Figure 24 illustrates the Brier-scores of all fully connected network variants. The lower the Brier-score, the better the probabilities learned. It is also possible to calculate the Brier-score for each class separately. In general, the fully connected networks have Brier-scores between 0–0.24. The calculations show that the Brier-scores vary from one type of pore to another. It seems obvious that the rarest pore classes (e.g. pore class A) have better Brier-scores than the more common pore classes (e.g. classes A and D). The more examples exist, the more discrepancies can occur. Nevertheless, the overall Brier-score shows a value between 0.107–0.108, with more neurons per hidden layer resulting in slightly better values. There is no clear dependence of the Brier-score on the number of hidden layers.

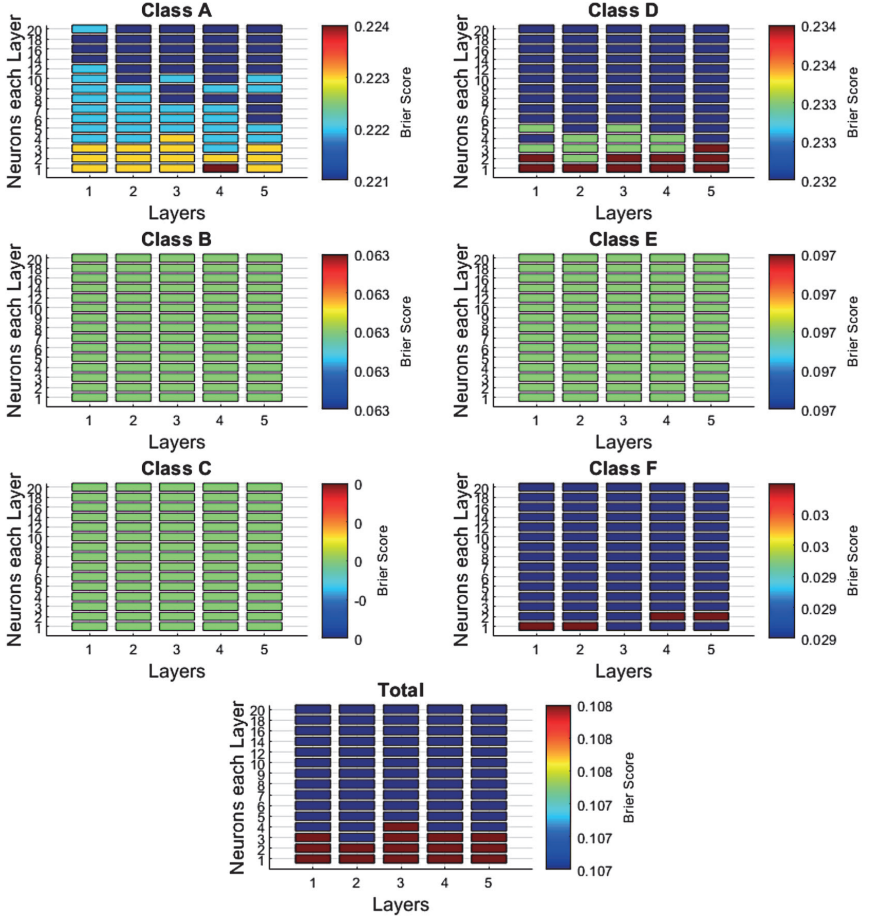


Figure 24: Brier-score for pore classes A–F and the total Brier-score in different fully connected neural networks (for PBF-LB/M prediction) with different numbers of hidden layers and neurons in each hidden layer

8.1.1.2. Generalisation Ability

According to the performance metrics AUC, Brier-score and cross-entropy, all neural network variants are able to make predictions. Neural networks with a larger number of neurons per layer seem to perform slightly better. To check the generalisation ability of the network beyond the known 32 parameter sets, an additional test was performed with 5 completely new parameter sets (Table 4). Figure 25 shows the additional generalisation test on unknown data for the PBF-LB/M pore class prediction. The CT pore data of 5 unknown parameter data sets were compared with the ML prediction. The deviations of the prediction of these comparisons are illustrated for each parameter set in different fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer. The generalisation check shows that each of the 75 neural networks predicts the new data differently. In general, the fully connected networks have prediction deviations between 0.41–13.44 %. For example, the neural network variant with 1 hidden layer and 6 neurons per layer has a mean prediction deviation of 13.44 % for predicting parameter set 4, while the same neural network variant has a much better deviation of 0.68 % for predicting parameter set 3. The neural network variant with 1 hidden layer and 6 neurons per layer is an example of a poor generalisation ability. This means that this neural network does not learn the real behaviour of the pore formation based on the parameter inputs scanning speed, layer thickness and hatch distance. The best generalisation ability is present in the neural network with 1 hidden layer and 9 neurons per layer. This network shows a mean prediction deviation of 1.04 % over all pore class predictions in all tested parameter sets. An overview of the PBF-LB/M pore class prediction for all 5 additional parameter sets using the best generalised network is shown in Figure 26. The orange bars represent the measured CT scans including the general CT measurement tolerance. Each parameter set was represented by 3 specimens. The CT measurement tolerance for each pore class (4.29 % (class A), 1.01 % (class B), 0.01 % (class C), 5.30 % (class D), 3.15 % (class E), 2.26 % (class F)) was determined by the standard deviations of these 3 specimens over all 32 parameter sets. The predictions (blue bars) agree almost perfectly with the measured pore type distribution (orange bars). Even the deviations between prediction and measurement are mostly within the CT measurement tolerances. The generalisation ability, which is the most important characteristic of a neural network, is achieved with a mean prediction deviation of 1.04 % over all pore class predictions.

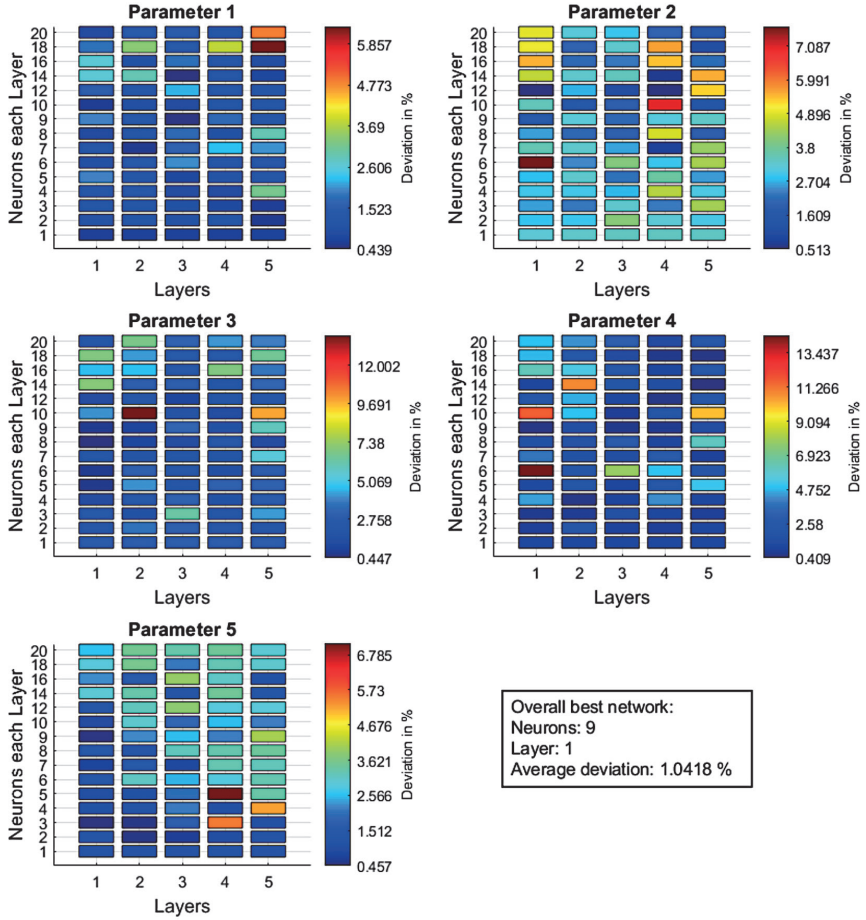


Figure 25: Additional generalisation test on unknown data for the PBF-LB/M pore class prediction. 5 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer

It is important to emphasise that even if all 5 sets of unknown parameters were predicted excellently, this cannot be transferred to all possible cases of unknown parameters. The results are only valid for the shown generalisation check. Nevertheless, the results reflect the real behaviour of the pore formation in the PBF-LB/M process quite well.

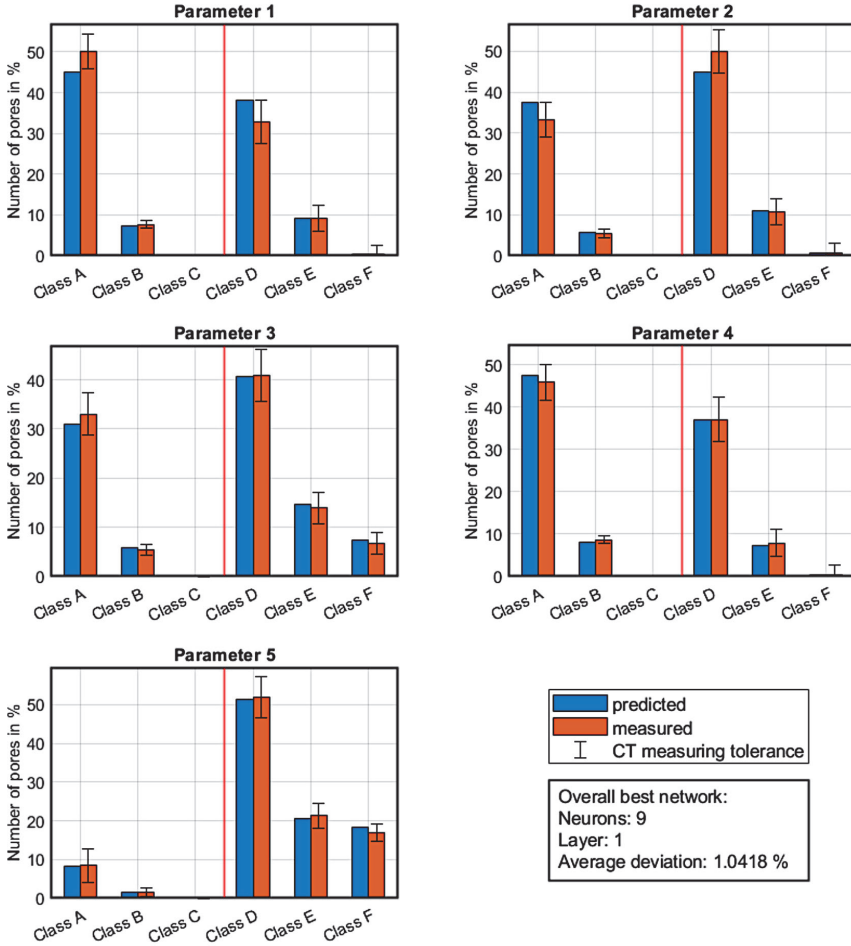


Figure 26: Illustration of the PBF-LB/M pore class prediction results of the best fully connected network using the example of 5 unknown parameter data sets (additional testing)

In addition to the fully connected network, the same analysis was carried out for the separated network design. The differences between fully connected and separated networks are described in chapter 4.3. The results of the separated neural networks can be found in the Appendix A.4. The summary of hyperparameter optimisation and model choice for both networks (fully connected and separated) is listed in Table 10. The performance metrics of both network designs are comparable, only the generalisation ability of the fully connected network is better. The

fully connected network with 1 hidden layer and 9 neurons per layer is used for all further predictions of PBF-LB/M parameters or pore types.

Model Architecture	Performance Metrics					Generalisation check
	Brier-Score	AUC (All-class Average)	Training Set (Cross-entropy)	Test Set (Cross-entropy)	Validation Set (Cross-entropy)	Prediction Deviation Average (%)
Fully Connected	0.107	0.628	0.199	0.199	0.198	1.04
Separated	0.107	0.638	0.199	0.199	0.198	1.24

Table 10: Summary of hyperparameter optimisation and model choice (PBF-LB/M pore type prediction)

8.1.2. Fully Connected ANN Model for Part Density

Part density can also be predicted using a neural network. Therefore, 96 part densities from 96 cylindrical specimens were measured using the Archimedes principle. A total of 864 part densities from the measurements and data extensions formed the part density database. Further information can be found in chapter 4.1.

8.1.2.1. Performance Metrics – CoD, MSE

The definition of CoD and MSE is summarised in chapter 2.3.8. Supervised learning methods can be divided into regression and classification algorithms. While the prediction of pore types (chapter 8.1.1) is a classification problem, the prediction of part densities is a regression problem. The main difference between regression and classification algorithms is the type of output data. Regression algorithms are used to predict continuous values (e.g. part densities), whereas classification algorithms are used to classify discrete values (e.g. pore types). Further information can be found in chapter 2.3.5 and chapter 2.3.8. Figure 27 shows the CoD and MSE colour maps for all 75 fully connected network variants. Unlike the mean squared error metric, the higher the CoD, the better the performance of the model. The MSE of the training (70 %), validation (15 %) and test (15 %) data set show values between 0.005–2.96 %², with more neurons per hidden layer resulting in better values. The CoD metric demonstrates the same tendency as the MSE. The CoD values range from -0.004–0.997.

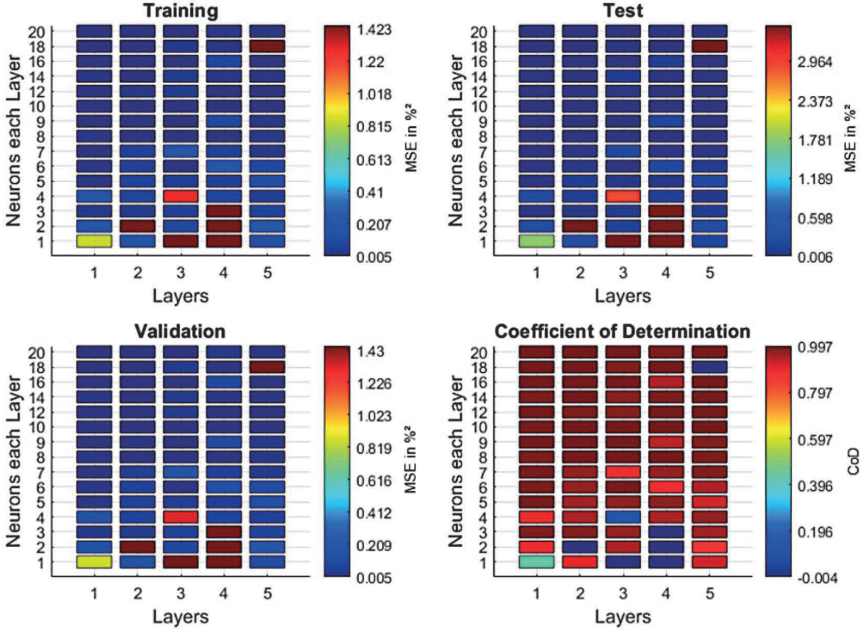


Figure 27: MSE for the training, test and validation data set as well as CoD in different fully connected neural networks (for PBF-LB/M part density prediction) with different numbers of hidden layers and neurons in each hidden layer

8.1.2.2. Generalisation Ability

Figure 28 shows the additional generalisation test on 5 unknown parameter sets. The part densities resulting from the 5 unknown parameter data sets were compared with the ML prediction. The deviations of these comparisons are illustrated for each parameter set in different fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer. The fully connected networks have prediction deviations between 0.006–6.78 %. Each of the 75 neural networks predicts the new data slightly differently. The best generalisation ability is present in the neural network variant with 2 hidden layer and 9 neurons per layer. This network has a mean prediction deviation of 0.198 % over all tested parameter sets. An overview of the part density prediction for all 5 additional parameter sets using the best generalised network is illustrated in Figure 29. The

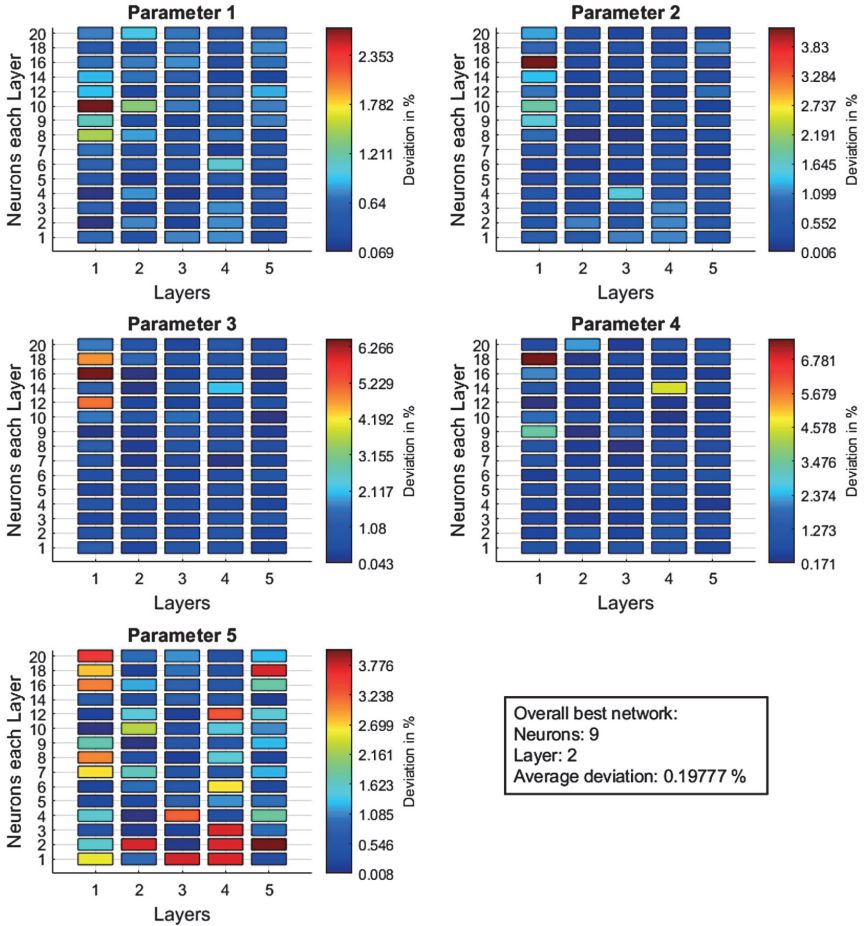


Figure 28: Additional generalisation test on unknown data for the PBF-LB/M part density prediction. 5 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer

orange bars represent the measured part densities including the general Archimedes measurement tolerance. Each parameter set was represented by 3 specimens. The Archimedes measurement tolerance (0.07 %) was determined by the standard deviations of these 3 specimens over all 32 parameter sets. The predictions (blue bars) always show slightly lower values than the measured part densities (orange bars). Furthermore, the deviations between prediction and measurement are not within the Archimedes measurement tolerances. Despite the small

deviations, the results are a good representation of the real behaviour of the part density in the PBF-LB/M process.

Note that the results are only valid for the shown generalisation check and cannot be transferred to all possible cases of unknown parameters. The model performances of the training, validation and test data as well as the regression plot of the best fully connected network (2 hidden layers and 9 neurons per layer) are visualised in the Appendix A.5. The summary of the hyperparameter optimisation and model choice for the fully connected network is listed in Table 11. The fully connected network with 2 hidden layers and 9 neurons per layer is used for all further predictions of PBF-LB/M parameters based on part densities.

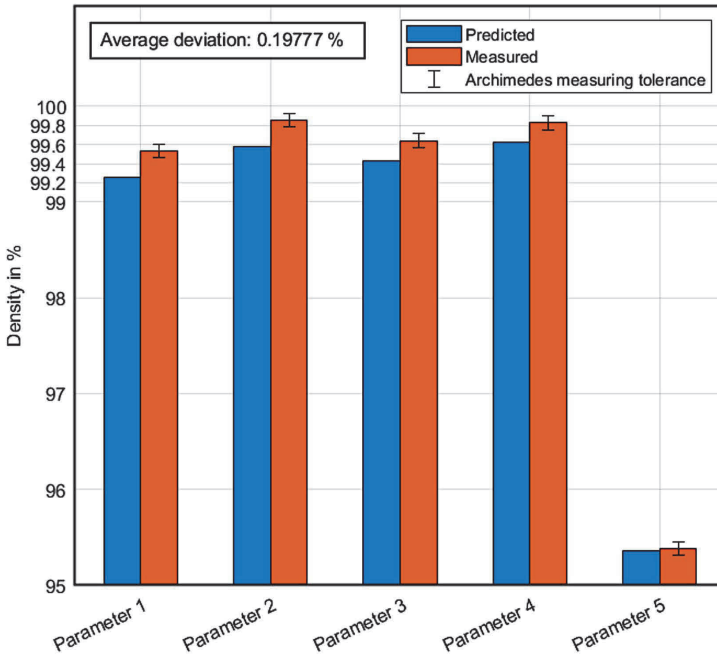


Figure 29: Illustration of the PBF-LB/M part density prediction results of the best fully connected network using the example of 5 unknown parameter data sets (additional testing)

Model Architecture	Performance Metrics				Generalisation check
	Training Set (MSE in % ²)	Test Set (MSE in % ²)	Validation Set (MSE in % ²)	CoD	Prediction Deviation Average (%)
Fully Connected	0.011	0.011	0.011	0.99	0.198

Table 11: Summary of hyperparameter optimisation and model choice (PBF-LB/M part density prediction)

8.2. Parameter Prediction (PBF-LB/M)

The best networks for PBF-LB/M were selected through a hyperparameter optimisation process, including performance metrics and the generalisation checking. These networks can predict several million combinations of process parameters based on the pore types and the part density. All the neural networks were trained within a typical parameter range for PBF-LB/M using aluminium alloys. These ranges were also used for the following parameter predictions. Let's assume that the scanning speed can be set in 750 possible steps (1000 mm/s to 1750 mm/s in 1 mm/s increments), the hatch distance in 320 possible steps (0.12 mm to 0.2 mm in 0.00025 mm increments) as well as the layer thickness in 240 possible steps (30 μ m to 90 μ m in 0.25 μ m increments). This would result in 57,600,000 predictable parameter combinations including the corresponding pore type distributions and part densities. It is obvious that not all possible cases can be visualised. Therefore, the 5 unknown parameter cases from the generalisation check (Table 4) will be used for the following prediction example. Only one parameter is varied, while the others remain constant. In this way 6550 prediction examples can be illustrated.

Figure 30, Figure 31 and Figure 32 show the prediction examples for all pore classes A–F as well as the part densities. As mentioned above, the process parameters that are not varied on the x-axis of the plots remain constant for the 5 examples. Besides the predictions, all measured values from the 5 parameter sets are visualised. The pore class predictions have a mean prediction deviation of 1.04 % over all pore class predictions in all tested parameter sets. The prediction of part density shows a mean prediction deviation of 0.198 % over all tested parameter sets. In general, there are completely different trends for different parameter settings. This is due to a complex interaction between porosity formation and process parameters. The pore analyses in publication II (Nudelis et al. [17]) showed that

the pore formation can be well described by the introduced volumetric energy density (VED). The definition of the VED is explained in chapter 2.1. The VED calculations are given in Table 4. Hence, the VED of the 5 measured parameter sets are used to facilitate the interpretation of the prediction results. The highest VED occurred for the parameter variation 1 (69.72 J/mm^3 , highlighted in blue). Parameter variation 5 (highlighted in red) had the lowest VED at 15.48 J/mm^3 . Parameter set 2 (36.76 J/mm^3 , highlighted in black), followed by parameter variation 4 (34.72 J/mm^3 , highlighted in yellow) and parameter set 3 (23.04 J/mm^3 , highlighted in green) showed intermediate VED values. The higher the introduced VED into the powder bed, the fewer irregularly shaped pores (classes D–F) and the more spherically shaped pores (classes A–C) occur. This behaviour is also visible for the 5 measured parameter sets. Parameter variation 1 (69.72 J/mm^3 , highlighted in blue) shows a higher number of spherically shaped pores (classes A–C) and fewer irregularly shaped pores (classes D–F) than, for example, parameter variation 5 (highlighted in red) with 15.48 J/mm^3 . Interestingly, the black prediction (parameter set 2, $\text{VED}=36.76 \text{ J/mm}^3$) and the yellow prediction (parameter set 4, $\text{VED}=34.72 \text{ J/mm}^3$) have almost the same VED values, but they show slightly different pore type formations. There must also be other influences than the introduced energy (VED) that affect the pore formation.

Nevertheless, the predictions follow the same trends as the measured values. It is worth mentioning again that the trained network has never seen these 5 measured parameter sets. This means that the network works in terms of generalisation (based on these test parameter sets). Furthermore, it is interesting to look separately at the influence of the scanning speed, hatch distance and layer thickness. Figure 30 shows the 750 scanning speed predictions for all pore classes A–F as well as the part densities. Hatch distance and layer thickness remain constant.

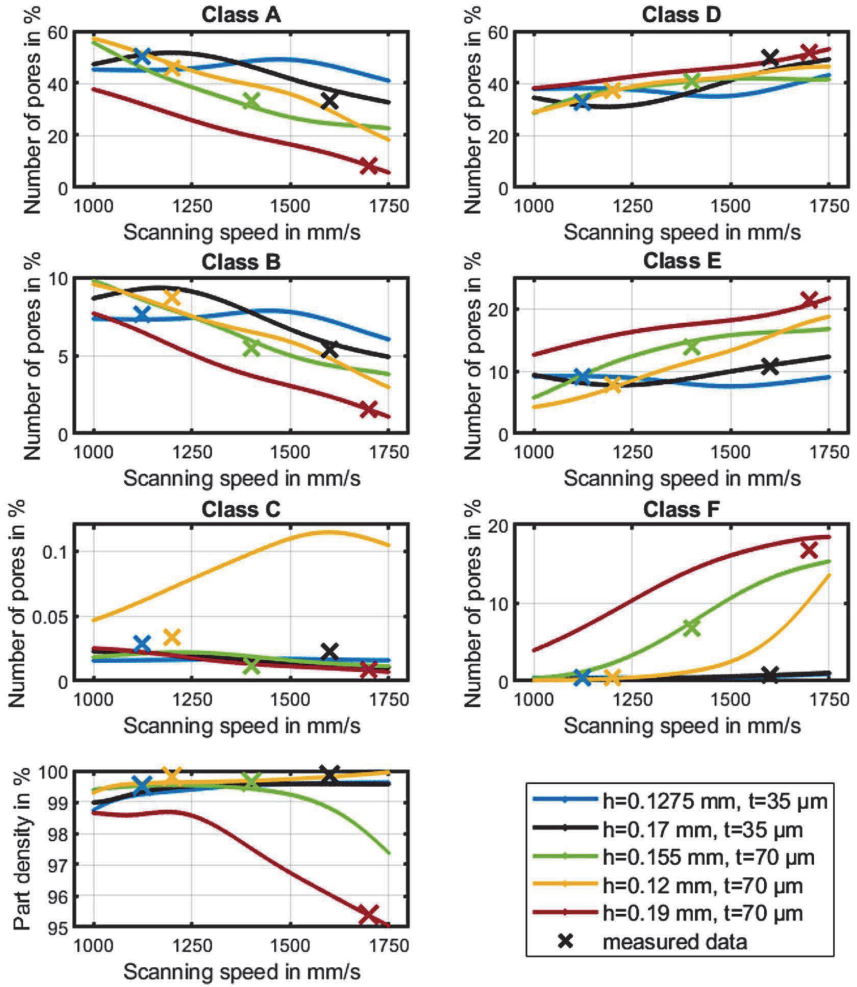


Figure 30: Scanning speed prediction for PBF-LB/M using the example of 5 unknown parameter data sets (additional testing)

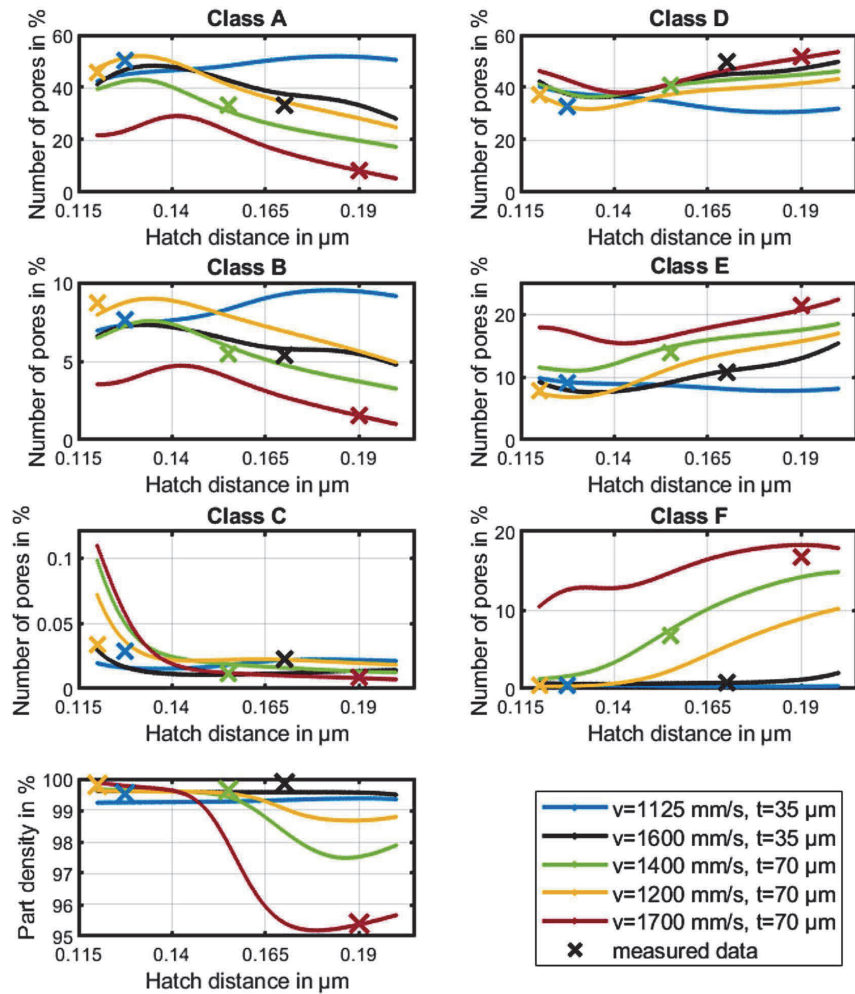


Figure 31: Hatch distance prediction for PBF-LB/M using the example of 5 unknown parameter data sets (additional testing)

In addition to the aforementioned pore formation tendencies with increasing or decreasing scanning speed (corresponding to an increase or decrease in VED), the simultaneous change in part density is of interest. While parameter sets 1, 2 and 4 (blue, black and yellow predictions) show a small increase in part density with increasing scanning speed, parameter sets 3 and 5 (green and red predictions) behave in the opposite way. The part density predictions also seem to follow the changes in VED. However, the measured values indicate that there must be also other influences than the introduced energy into the powder bed. The measured value from parameter set 1 (69.72 J/mm^3 , highlighted in blue) has a much higher VED than parameter set 4 (34.72 J/mm^3 , highlighted in yellow). Despite this, the lower VED value (34.72 J/mm^3) indicates higher part densities.

It is also worth noting the behaviour of the part densities in parameter case 2 (black prediction). The results in Figure 30, Figure 31 and Figure 32 clearly show an increasing or stagnating behaviour of the part density with increasing scanning speeds and hatch distances, while the part densities start to drop sharply from a layer thickness of about $50 \text{ }\mu\text{m}$.

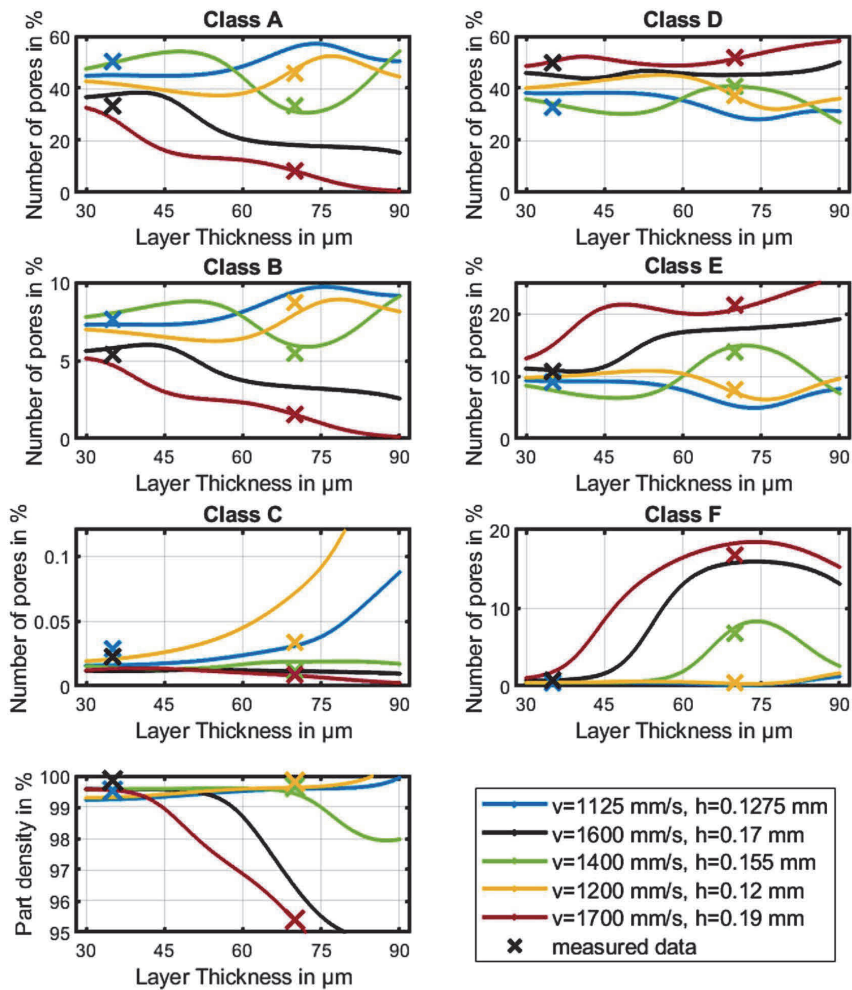


Figure 32: Layer thickness prediction for PBF-LB/M using the example of 5 unknown parameter data sets (additional testing)

8.3. Hyperparameter Optimisation and Model Choice (HIP)

8.3.1. Fully Connected ANN Model for Pore Types

All 1,489,857 pores from 8 HIP process parameter variations (Table 5) collected in 48 cylindrical specimens were used to train the following HIP neural networks. Furthermore, the pore data were collected using the pore tracing method described in publication III (Nudelis et al. [18]) and subsequently classified using the classification method described in publication I (Nudelis et al. [16]).

8.3.1.1. Performance Metrics – AUC, Brier-Score, Cross-Entropy

Figure 33 shows the AUC colour maps for each pore type A–F for all 75 fully connected HIP network variants. The definition of the ROC-curve and the resulting AUC metric are summarised in chapter 2.3.8. In general, the fully connected networks have AUC values between 0–0.95. An AUC value of 1 describes a perfect classifier, while a value of AUC = 0.5 indicates a random classifier. An AUC = 0 means that no classification was correctly predicted or no data was available. The results show that the AUC values differ from one pore type to another. Note that the pore types are collected in an imbalanced data set. All classified pores from all 8 parameter sets (before and after HIP) are visualised in the Appendix A.3. Before HIP, the small pore types A and D are present in larger numbers than the larger pore classes B, C, E, F. After all HIP treatments, the pores were mainly closed or transformed to pore class D. After HIP, a small number of pores were present as pore classes E and F. The classes B and C were completely closed (no data available). That's why all network variations for pore classes B and C have an AUC = 0. The pore classes A, D, E and F as well as the closed pores, show high AUC values up to 0.95. It seems obvious that more neurons per hidden layer lead to better AUC values for the pore types A, D, E and the closed pores. Only pore class F seems to be more independent of the number of neurons. There is no clear dependence of the AUC on the number of hidden layers.

Figure 34 shows the Brier-scores of all 75 fully connected HIP network variants. The lower the Brier-score, the better the probabilities learned. It is also possible to calculate the Brier-score for each class separately, as well as for the closed pores. In summary, the fully connected networks have Brier-scores between 0–0.055. The results show that the Brier-score values differ from one class to the other class. The minority pore classes remaining after HIP (classes A, E, F) tend to have better Brier-scores than the majority pore class D. The more examples exist, the more discrepancies can occur. Interestingly, pore class F shows a perfect prediction ability (also a Brier-score = 0) for all tested network variations. Due to a lack

of data for the pore classes B and C after HIP, no predictions were made and the Brier-score is 0. The overall Brier-score shows a value between 0.015–0.016, with more neurons per hidden layer resulting in slightly better values. There is no clear dependence of the Brier-score to the number of hidden layers.

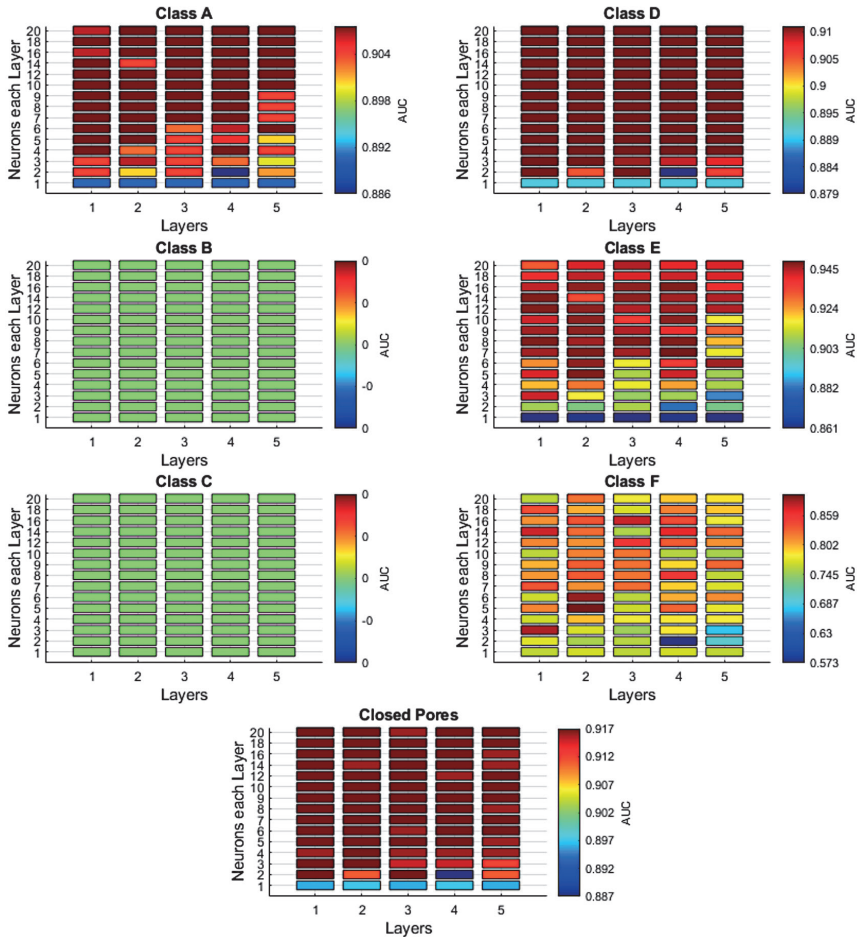


Figure 33: AUC for pore classes A–F and closed pores in different fully connected neural networks (for HIP prediction) with different numbers of hidden layers and neurons in each hidden layer

The Brier-score metric was calculated based on the independent test data set (15 %) from the 8 parameter sets. This means that the Brier-score checks the generalisation ability of the network based on this test data set. Most likely, the test data set is not variable enough compared to the training and validation data set to check the generalisation ability beyond the 8 parameter variations. The same situation occurred for the PBF-LB/M networks in chapter 8.1.1.

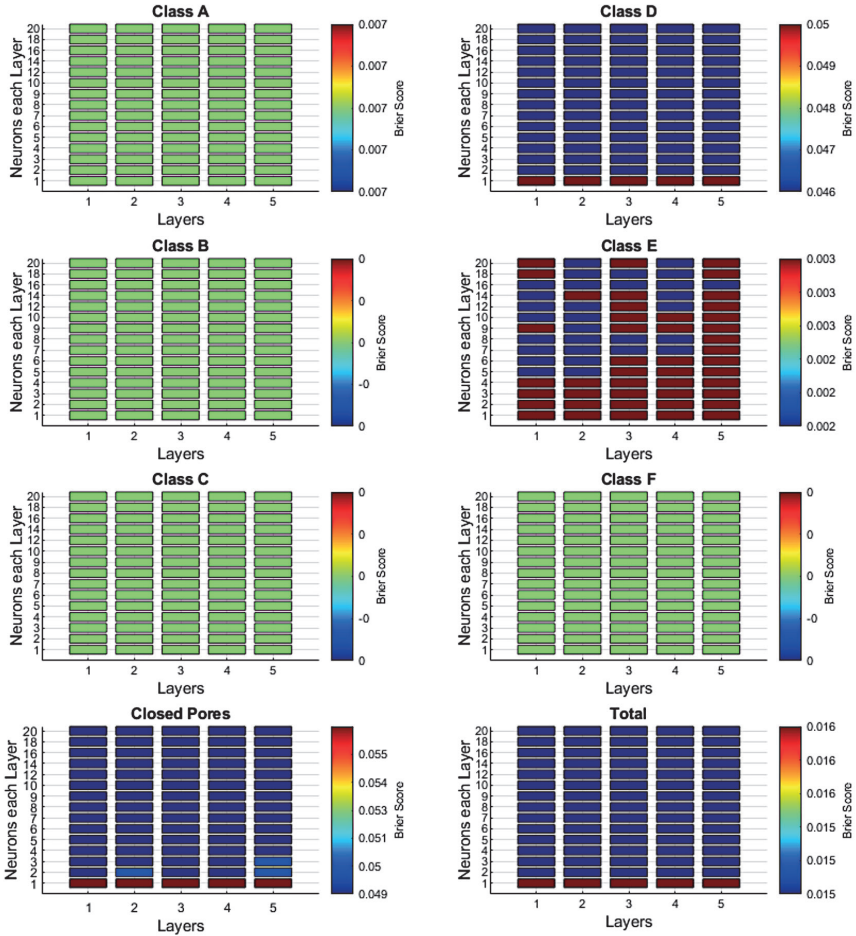


Figure 34: Brier-score for pore classes A–F as well as closed pores and the total Brier-score in different fully connected neural networks (for HIP prediction) with different numbers of hidden layers and neurons in each hidden layer

Figure 35 shows that the cross-entropy for the training (70 %), validation (15 %) and test (15 %) data sets are very similar. Hence, the Brier-score only checks how accurately the network predicts the known 8 parameter sets with new but similar data information. Therefore, a generalisation check beyond these known 8 parameter sets is performed with an additional test data set using complete unseen parameters (chapter 8.3.1.2).

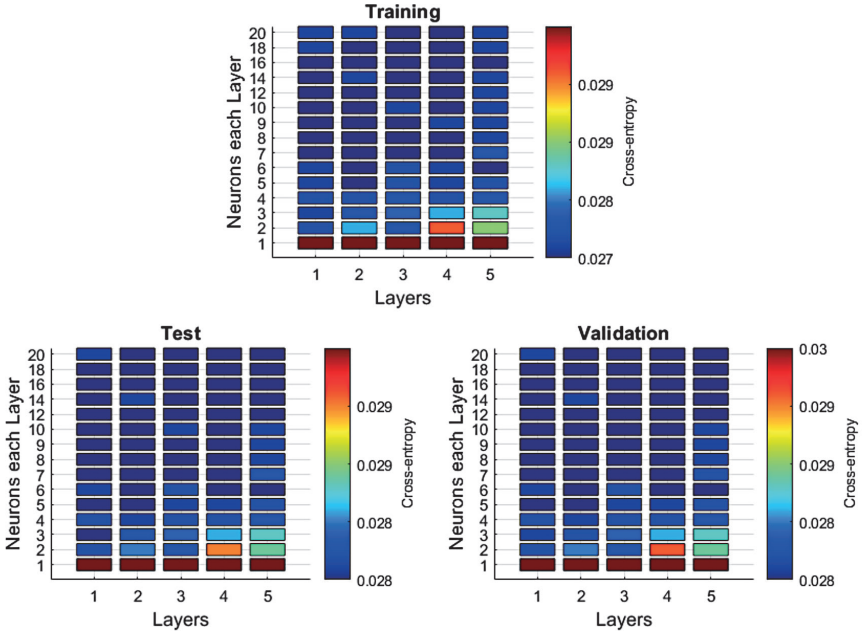


Figure 35: Cross-entropy for the training, test and validation data set in different fully connected neural networks (for HIP pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

8.3.1.2. Generalisation Ability

The previous analysis of the performance metrics AUC, Brier-score and cross-entropy showed that all neural network variants are able to predict pore classes as well as the closed pores. In addition, Figure 36 shows the generalisation test on unknown data for the HIP pore class prediction. The CT pore data of 3 unknown HIP parameter data sets were compared with the ML prediction. The deviations of these comparisons are illustrated for each parameter set in different fully connected neural networks with different numbers of hidden layers and neurons in

each hidden layer. The results show that each of the 75 neural network variants predicts the new data differently. In summary, the fully connected networks have prediction deviations between 0.0004–19.71 %. It seems obvious that fully connected neural networks with only 1 neuron per layer are generally insufficient in terms of generalisation. Another example of poor generalisation is the network with 4 hidden layers and 18 neurons per layer. This variant of the network shows quite high mean prediction deviations for all new parameter predictions of 14.44 % (parameter set 1), 8.98 % (parameter set 2) and 9.41 % (parameter set 3). This means that this neural network does not learn the real behaviour of the pore closure mechanisms based on the parameter inputs pressure, temperature and time accurately enough. The best generalisation ability is observed in the neural network with 2 hidden layers and 20 neurons in each layer. This network shows a mean deviation of the prediction of 0.56 % over all pore classes and pore closure predictions in all tested parameter sets.

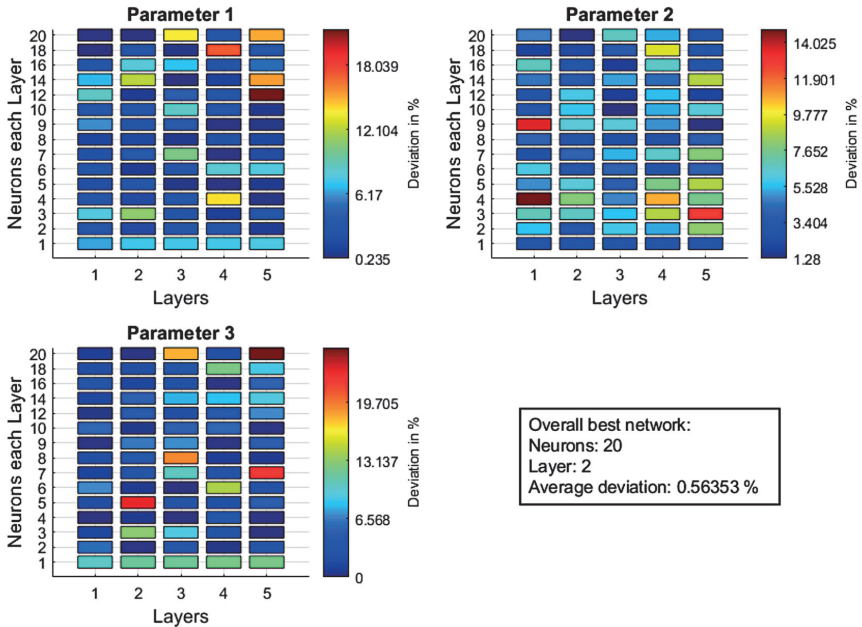


Figure 36: Additional generalisation test on unknown data for the HIP pore class prediction. 3 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer

An overview of the HIP pore class prediction for all 3 additional parameter sets using the best generalised network is shown in Figure 37. The orange bars represent the CT scans including the general CT measurement tolerance for each pore class after HIP (0.24 % (class A), 0 % (class B), 0 % (class C), 0.30 % (class D), 0.17 % (class E), 0.0007 % (class F), 0.38 % (closed pores)). The CT measurement tolerance for all hipped pore classes was determined by the standard deviation of 6 specimens over all 8 parameter sets. The predictions (blue bars) agree almost perfectly with the measured pore type distribution (orange bars). Note that even though all 3 sets of unknown parameters were predicted excellently, this cannot be transferred to all possible cases of unknown parameters. The results are only valid for the shown generalisation check. Nevertheless, the results of the generalisation check show that the network reflects the real behaviour of the HIP process well.

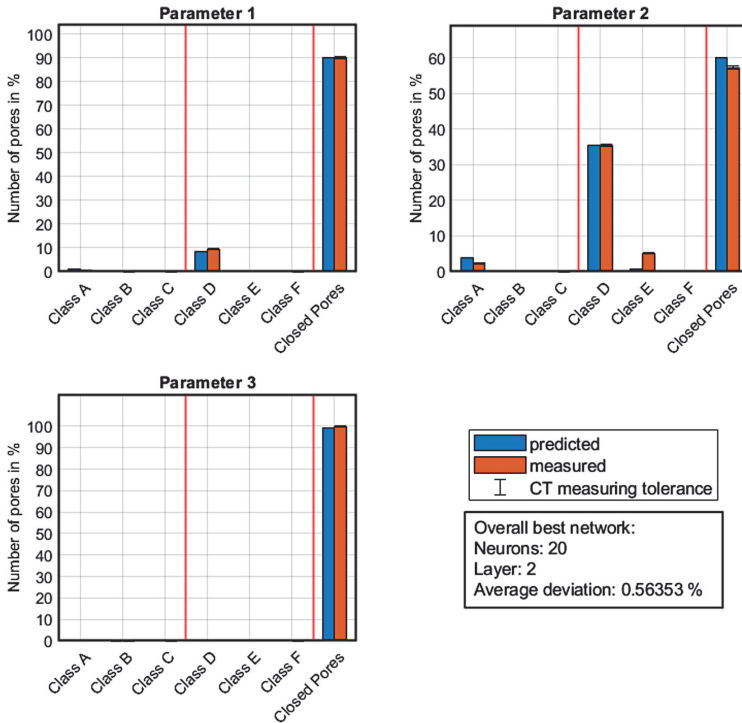


Figure 37: Illustration of the HIP pore class prediction results of the best fully connected network using the example of 3 unknown parameter data sets (additional testing)

In addition to the HIP fully connected network, the same analysis was carried out for the HIP separated network design. The differences between fully connected and separated networks are described in chapter 4.3. The results of the separated neural networks can be found in the Appendix A.6. The summary of hyperparameter optimisation and model choice for both networks (fully connected and separated) is listed in Table 12. The performance metrics of both network designs are comparable, only the generalisation ability of the fully connected network is better. The fully connected network with 2 hidden layer and 20 neurons per layer is used for all further predictions of HIP parameters or pore types.

Model Architecture	Performance Metrics					Generalisation check
	Brier-Score	AUC (All-class Average)	Training Set (Cross-entropy)	Test Set (Cross-entropy)	Validation Set (Cross-entropy)	Prediction Deviation Average (%)
Fully Connected	0.015	0.892	0.028	0.028	0.028	0.56
Separated	0.015	0.887	0.028	0.028	0.028	0.83

Table 12: Summary of hyperparameter optimisation and model choice (HIP pore type prediction)

8.3.2. Fully Connected ANN Model for Hardness

In addition to the pores, the hardness was also determined in order to train a neural network. A total of 28 samples from 8 parameter variations (Table 5) as well as reference samples without any HIP treatment were analysed. A total of 756 hardness values from the measurements and data extensions formed the database for the following network training. Further information can be found in chapter 4.1.

8.3.2.1. Performance Metrics – CoD, MSE

Figure 38 shows the CoD and MSE colour maps for the 75 fully connected network variations. On the one hand, the higher the CoD, the better the performance of the model. On the other hand, the network works better with lower MSE values. The MSE of the training (70 %), validation (15 %) and test (15 %) data set show values between 0.32–16.47 HBW², with fewer hidden layers and more neurons per hidden layer resulting in better values. The CoD metric demonstrates the same tendency as the MSE. The CoD values are between 0.96–0.99.

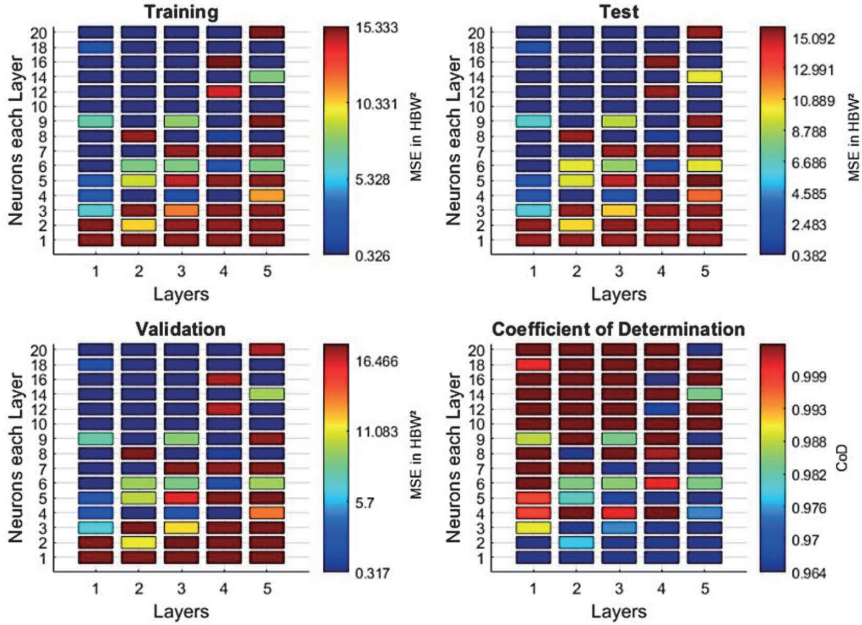


Figure 38: MSE for the training, test and validation data set as well as CoD in different fully connected neural networks (for HIP hardness prediction) with different numbers of hidden layers and neurons in each hidden layer

8.3.2.2. Generalisation Ability

The hardness resulting from the 3 unknown parameter data sets was also compared with the ML prediction. Figure 39 illustrates the deviations of these comparisons for each parameter set in different fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer. The trained networks show prediction deviations between 0.05–39.43 HBW. Each of the 75 neural networks predicts the new data in a different way. The deviations for parameter set 3 are the highest. It should be noted that the parameter sets 2 and 3 are further away from the known parameter data range than parameter set 1. The known parameter range of the networks is between 30 min to 90 min (treatment time), 300 bar to 2000 bar (pressure) and 480 °C to 540 °C (temperature). All parameter sets for the generalisation check are new data for the trained networks. However, parameter set 2 (200 bar) and parameter set 3 (15 min) are also outside the known parameter range of all data. Interestingly, the networks show a better generalisation ability for an unusual pressure change than for the treatment time.

Nevertheless, there are also network variants (mostly with many neurons per layer) that predicted all parameter changes with a small deviation.

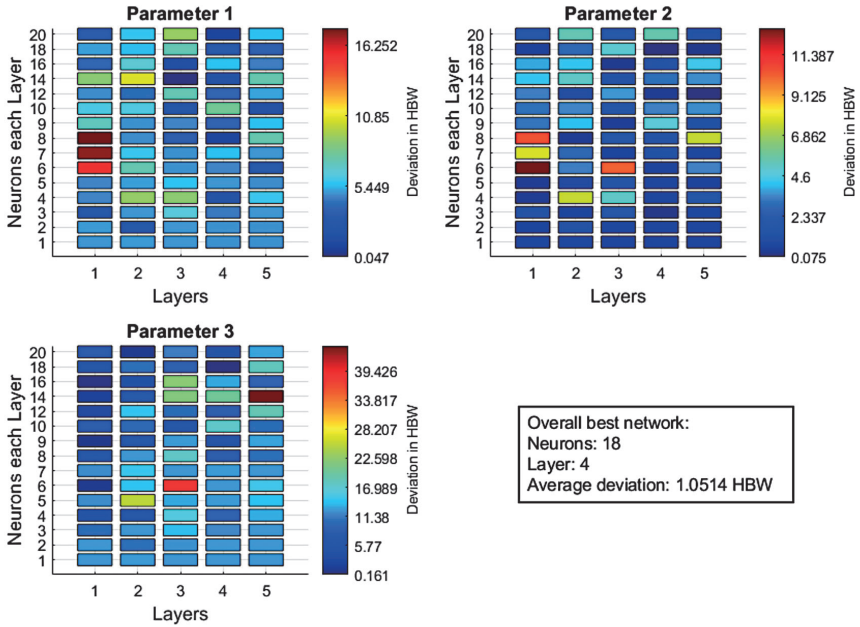


Figure 39: Additional generalisation test on unknown data for the HIP hardness prediction. 3 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained fully connected neural networks with different numbers of hidden layers and neurons in each hidden layer

The best generalised network with a mean prediction deviation of 1.05 HBW has 4 hidden layers and 18 neurons within this layer. The hardness prediction for the 3 unknown parameter sets is shown in Figure 40. The orange bars represent the measured hardness values including the general hardness measurement tolerance (± 0.45 HBW). Further information on the determination of the general hardness measurement tolerance can be found in chapter 4.1. The predictions (blue bars) always show slightly lower values than the measured hardness values (orange bars). Moreover, the deviations between prediction and measurement are not always within the measurement tolerances. Apart from the slight underestimation of the neural network model, the real behaviour of the hardness after HIP treatment is still represented. As with all shown generalisation checks, the results are only valid for the tested parameter sets and cannot be transferred to all possible unknown parameter cases. The model performances of the training, validation

and test data as well as the regression plot of the best fully connected network (4 hidden layers and 18 neurons per layer) are given in the Appendix A.7. The summary of the hyperparameter optimisation and model choice for the fully connected hardness network is listed in Table 13. This selected network with 4 hidden layers and 18 neurons per layer is used for all further HIP parameter predictions based on the hardness.

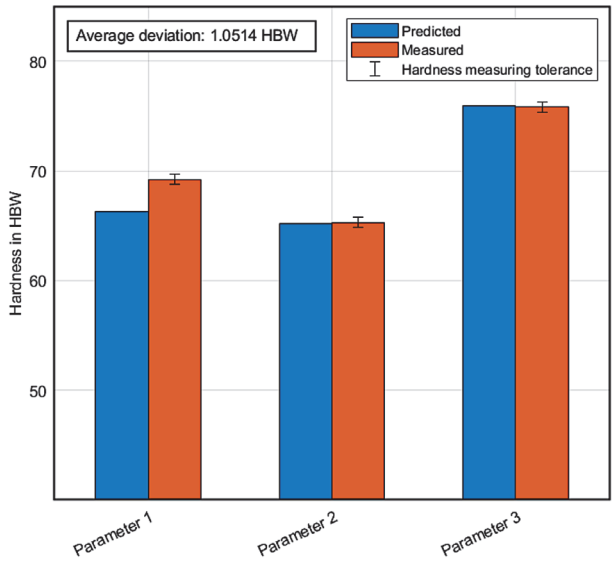


Figure 40: Illustration of the HIP hardness prediction results of the best fully connected network using the example of 3 unknown parameter data sets (additional testing)

Model Architecture	Performance Metrics				Generalisation check
	Training Set (MSE in HBW ²)	Test Set (MSE in HBW ²)	Validation Set (MSE in HBW ²)	CoD	Prediction Deviation Average (HBW)
Fully Connected	0.33	0.38	0.32	0.99	1.05

Table 13: Summary of hyperparameter optimisation and model choice (HIP hardness prediction)

8.4. Parameter Prediction (HIP)

The best neural networks for the HIP predictions were selected using a hyperparameter optimisation, including performance metrics and generalisation checks. Several million combinations of HIP process parameters can be predicted based on the pore classes before and after HIP as well as the hardness. All neural networks were trained within a possible parameter range for AlSi10Mg HIP applications. The neural networks learned pressure in a range from 300 bar to 2000 bar, temperature in a range from 480 °C to 540 °C as well as the treatment time in a range from 30 min to 90 min. Furthermore, the generalisation checks used a slightly extended range of parameters outside the known range. It is obvious that not all possible cases can be visualised in this chapter. Therefore, the 3 unknown parameter cases from the generalisation check (Table 6) were used for the following prediction examples, including an extended parameter range.

Let's assume that the pressure can be adjusted in 1820 possible steps (180 bar to 2000 bar in 1 bar increments), the temperature in 100 possible steps (450 °C to 550 °C in 1 °C increments) as well as the treatment time in 90 possible steps (10 min to 100 min in 1 min increments). This would result in 16,380,000 predictable HIP parameter combinations, including corresponding pore distributions and hardness values. Using only the learned parameter range, 6,120,000 cases can be predicted. In addition to the process parameters, the initial pore distribution prior to HIP is relevant to the HIP treatment result. In this work, all HIPed specimens were made with the same PBF-LB/M parameters (details in chapter 4.1). The initial pore distribution was kept constant at 40.69 % (class A), 9.14 % (class B), 0.02 % (class C), 36.31 % (class D), 13.34 % (class E) and 0.49 % (class F). Figure 41, Figure 42 and Figure 43 illustrate the prediction examples for all pore classes A–F and the closed pores during the presented HIP parameter cases. The process parameters that are not varied on the x-axis of the plots remain constant for the 3 examples. In addition, all measured values from the 3 parameter sets are shown. It seems important to repeat that the pore network has a mean prediction deviation of 0.5635 % over all pore class predictions in all tested parameter sets. Irrespective of the existing pore class, all class predictions show a clear downward trend with higher pressure, temperature and time values and the number of closed pores simultaneously increases. Furthermore, the predictions follow the same trends as the measured values.

Note that the trained network has never seen these 3 measured parameter sets, indicating a good generalisation ability (based on these tested parameter sets). The measured values of parameter set 2 (highlighted in black) show the highest deviations compared to the predictions. However, the deviations do not lead to a large distortion of the reality with respect to the overall pore distribution. Moreover,

the number of pores and the trends shown by the predictions are in agreement with the results presented in publication III (Nudelis et al. [18]).

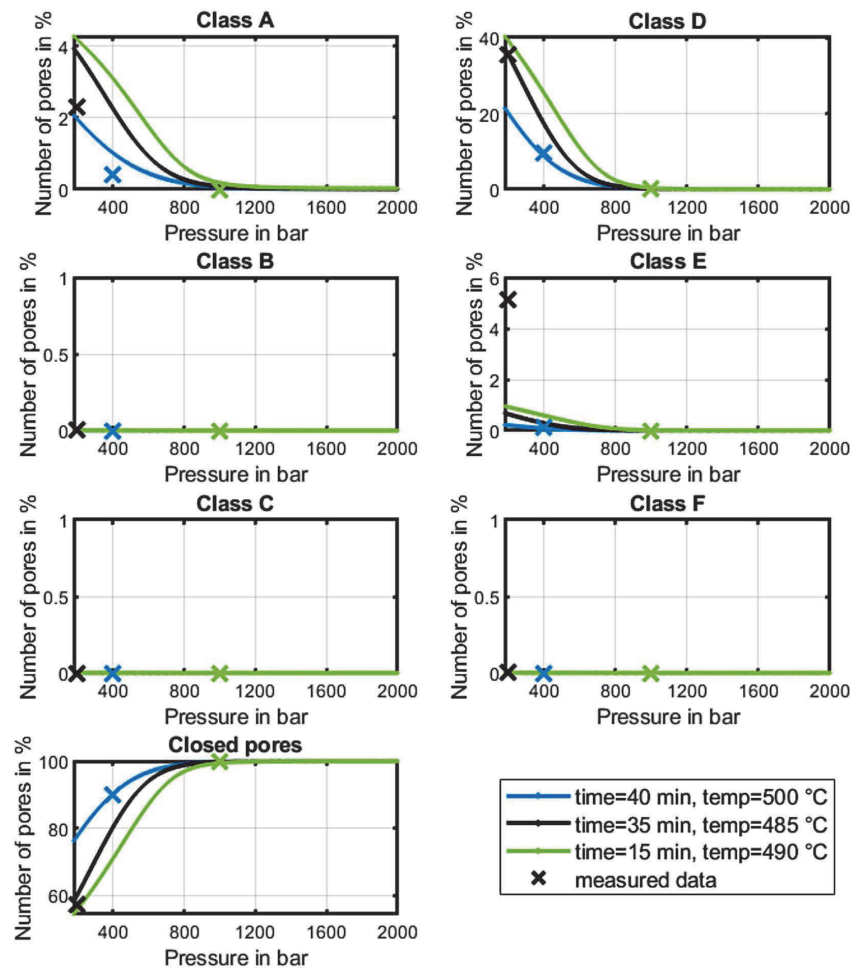


Figure 41: Pressure prediction for HIP using the example of 3 unknown parameter data sets (additional testing)

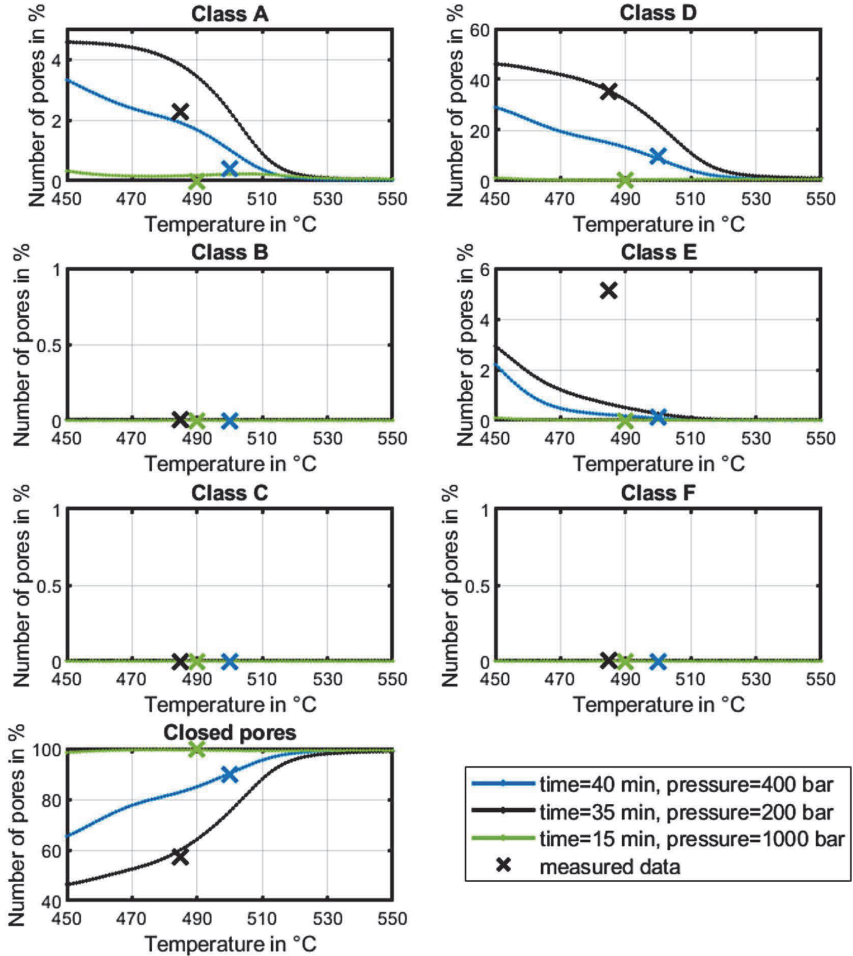


Figure 42: Temperature prediction for HIP using the example of 3 unknown parameter data sets (additional testing)

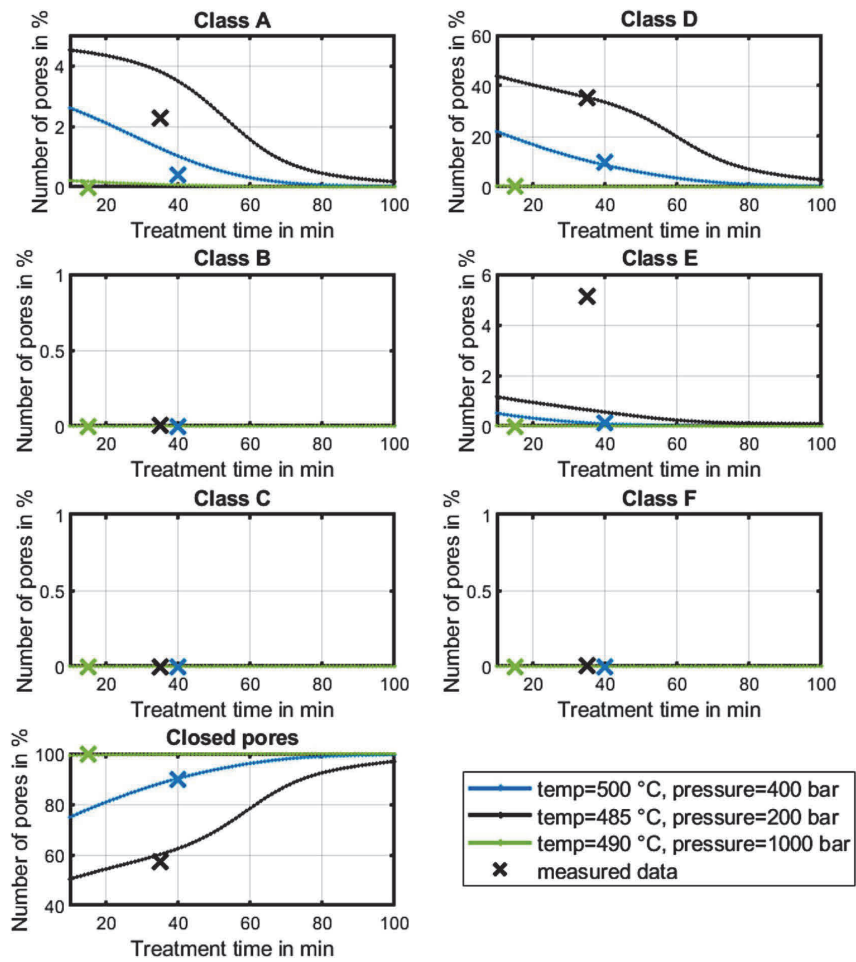


Figure 43: Treatment time prediction for HIP using the example of 3 unknown parameter data sets (additional testing)

The hardness prediction in Figure 44 has a mean prediction deviation of 1.05 HBW over all tested parameter sets. It is interesting to note that the temperature has the greatest influence on the hardness during the HIP treatment. The hardness before HIP was around 120 HBW, which dropped to values between 60–80 HBW depending on the HIP treatment settings. Pressure and time did not appear to have a major effect on hardness. As for the porosity prediction, the trained network never saw these 3 measured parameter sets, which indicates a good generalisation ability (only assessable on these tested parameter sets).

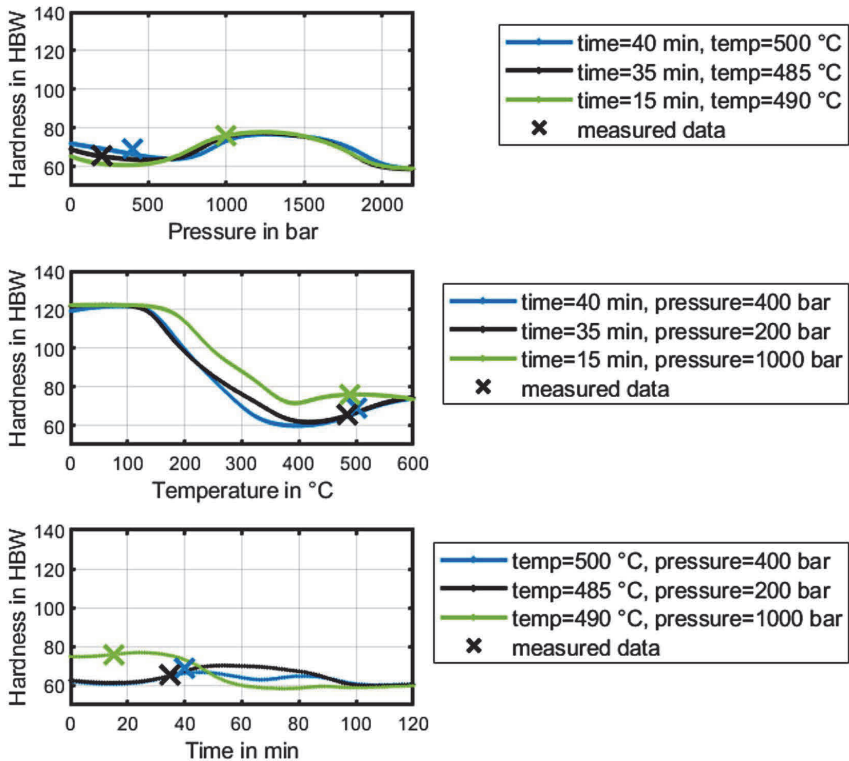


Figure 44: Hardness prediction for HIP using the example of 3 unknown parameter data sets (additional testing)

8.5. Machine Learning: Summary and Discussion of Findings

A total of 4,556,106 pores, 864 part densities and 756 hardness values were recorded to train the PBF-LB/M and HIP neural networks. All the raw pore data were pre-processed using the novel classification method (Nudelis et al. [16]) and the pore tracing method (Nudelis et al. [18]). Additional input was provided by part density and hardness measurements as well as data extension techniques. The goal of this project was to predict PBF-LB/M and HIP process parameters based on quality characteristics such as pore types, part densities and hardness values.

The influence of different numbers of hidden layers (1–5) and neurons (1–20) was investigated by hyperparameter optimisation using the grid search approach. Several performance metrics were used to evaluate the networks against each other. The area under the ROC curve (AUC), the Brier-score as well as the cross-entropy were chosen to evaluate the trained classification models. The coefficient of determination (CoD) and the mean squared error (MSE) were used to evaluate the trained regression networks. All models using pore data were built as a classification task, whereas the part density and hardness networks represent regression tasks. All regression and classification networks were successfully trained. The best PBF-LB/M networks showed in the generalisation checks an average prediction deviation of 1.04 % (pore type network) and 0.198 % (part density network), the best HIP networks performed with an average prediction deviation of 0.56 % (pore type network) and 1.05 HBW (hardness network).

In general, the results showed that more neurons per hidden layer led to better performance metrics and thus to better predictions. There was no clear dependence on the number of hidden layers. The performance metrics clarified how many hidden layers and neurons per layer are needed. Nevertheless, it remains to be discussed why the tested networks have similar performance metrics but still predict very differently in the generalisation checks. One explanation for this phenomenon could be the random nature of the trained networks. The 75 training sessions of each network type used the same division of trainings, test and validation data as well as the same parameters (hyperparameters were varied). But, each training is unique due to a random initialisation of weight and bias values. As a result, different neural networks trained on the same data input can produce different outputs. The reason for the random nature of the networks is caused by the used initialisation function, called Nguyen-Widrow initialisation [62], which generates random initial weights and biases each time. This also affects the way the network sets the weights in the next learning iterations.

On the one hand, the Nguyen-Widrow algorithm significantly reduces the training time [62–63]. On the other hand, it can also improve the performance metrics of the trained networks [63]. The weight and bias initialisation process is an important step in the development of an artificial neural network. A very thorough review of different initialisation methods can be found in Narkhede et al. [64]. Further investigations could examine the influence of different initialisation methods on the model performance and clarify the potential for improvement.

It is also important to note that the pore types were collected in an imbalanced data set. The small pore types A and D appear in greater numbers than the larger pore types B, C, E, F. Furthermore, the output describes a pore distribution in the form of a probability. Any manipulation of the original quantity of pore data could affect the final pore distribution. Hence, no data was removed from the original data set during the data pre-processing. Fernandez et al. [41] mentioned that class imbalance can result in a poor ability of the model to predict the minority classes. In our case, less data led to more discrepancies. The less data existed, the greater the dependence on the number of hidden layers and their neurons. In fact, the minority classes showed a greater dependency in the hyperparameter investigations. However, there were still several neural network variants with good generalisation ability to predict majority and minority classes. In addition, class binarisation techniques can be used to overcome the problem of imbalanced data [41]. Therefore, an adapted approach using separate neural lines for each output variable (e.g. pore class) was tried out (Appendices A.4. and A.6.). Interestingly, the performance metrics of the fully connected and separated network designs were comparable, only the generalisation ability of the fully connected network was better. The problem of imbalanced data does not seem to be an issue in this project.

The discussion, including the underlying publications [16–18], takes place in the following chapter 9.

9. Summary, Conclusion and Outlook

In the following chapter, the scientific contribution of this publication-based work will be reflected on the basis of the three underlying publications [16–18] and the machine learning results in relation to the state of the art.

9.1. Summary

Additive manufacturing (AM) using laser powder bed fusion (PBF-LB/M) has many advantages such as design freedom and sustainability. However, AM also experiences internal defects that limit the reproducibility of its quality. In the current state of laser powder bed fusion of Al alloys, porosity is an inevitable concomitant. As a result, PBF-LB/M has not been widely adopted in the high-tech industries such as aerospace, automotive or healthcare. Past research has focused extensively on determining the types and origins of pores in the PBF-LB/M process using Al alloys. This has resulted in a wealth of knowledge that can be used to further improve the technology. Furthermore, post-treatment technologies such as hot isostatic pressing (HIP) can help to remove pores and produce high-density and microstructurally homogeneous components.

The aim of this work is to develop a machine learning (ML) system to predict PBF-LB/M or HIP process parameters based on quality characteristics such as pore types, part densities and hardness values. Therefore, supervised learning methods such as artificial neural networks were considered as a solution approach. The development and training of such ML systems requires suitable data acquisition methods as well as a detailed understanding of the process. For this reason, the work was divided into two chapters. The first chapter focuses on the data acquisition, preparation and process analysis (all carried out in peer-reviewed publications), while the second chapter deals with the application of machine learning. The pore analysis (Nudelis et al. [17]) demonstrated that pores contain a lot of useful information about the used process parameters and the process conditions.

Pores can be seen as an individual process fingerprint. On the one hand, the novel pore classification (Nudelis et al. [16]) and pore tracing method (Nudelis et al. [18]) were able to convert the raw X-ray data into a usable data set for supervised learning applications. On the other hand, data extension techniques and the measurement of part densities and hardness values provided additional input to the ML

system. Several neural networks were successfully trained with the classified and processed data. The summary and discussion of the machine learning results are presented in chapter 8.5. The findings show that a small number of experiments and measurements can be sufficient to create neural networks with a good predictive ability. However, this requires sufficient data acquisition and preparation, which has been achieved through several analyses and developments, such as the novel classification and pore tracing algorithm.

9.2. Conclusion and Outlook

X-ray tomography has already proven its effectiveness in analysing defects in AlSi10Mg components [57–58]. However, the high information content has not been fully exploited due to a lack of evaluation methods. Several studies have attempted to classify the pores using different shape descriptors. Maskery et al. [65] used sphericity and aspect ratio, while Hastie et al. [66] tried dimensional descriptors based on the bounding box or the feret calliper method. They either used only 2D image analysis or examined 3D geometry in many specific shape classes. Nudelis et al. [16] showed that at least three shape indicators are necessary to define the 3-dimensional pore shape as accurately as possible. The combined use of sphericity, compactness and bounding-box factor led to a reduction in misclassifications. Furthermore, finite element analysis (FEA) and fracture mechanics calculations showed that two shape classes (spherical and irregular shaped) were sufficient in terms of criticality (failure due to high stress concentration). The novel classification method (Nudelis et al. [16]) classifies pores according to pore size (small, medium, large) and pore shape (spherical or irregular). In addition to all the advantages of computed tomography, it is important to discuss the technological limitations of X-ray scans and thus of the developed classification approach. The limiting factors can be the component size or material density, which can result in X-ray penetration issues. X-ray penetration problems can lead to a decrease in data quality and consequently to a loss of information [67]. Du Plessis et al. [67] mentioned higher voltage systems, beam filtration and optimised scanning parameters as possible actions against X-ray penetration problems. However, no limitations were identified for the used cylindrical specimen (10 mm in diameter and 18 mm in height) of AlSi10Mg. In addition, some work has criticised the CT technology for its limited scan resolution [68–69]. In this work, X-ray scans were taken with a minimum voxel size of $9.659 \mu\text{m}^3$. A typical minimum pore size requires at least three voxels to be accurately visualised [67], which means that only pores $> 30 \mu\text{m}$ were detectable. Generally speaking, large components (especially those made of a dense material) and a low resolution will result in a lack of pore data. These limitations must be taken into account when using CT and the developed pore classification method.

There is no doubt that process parameters play an important role in part quality [4,6,19,70]. However, part quality is determined by many more influences. Kokareva et al. [15] described that the final part quality is defined by powder characteristics, process parameters, machine equipment, finishing process as well as part geometries. In this work, only a few process parameters are included in the quality predictions. It seems obvious that further inputs need to be generated to improve the capabilities of the prediction models. Further discrepancies may occur due to a lack of information. For example, any change in powder characteristics such as flowability, bulk density or chemical composition or the choice of material or manufacturing technology, can lead to deviations between model predictions and reality. These models have only been trained on new AlSi10Mg powder from the same supplier, processed in SLM500 machines. Furthermore, it is expected that predictions closer to the known parameter data sets will generate better results than predictions in completely unknown parameter ranges. The checked generalisation ability within the range of known parameter sets (or slightly outside the range) showed almost perfect predictions. Nevertheless, the results are only valid for the shown generalisation checks.

Today, additive manufacturing is recognised for its flexibility, design freedom and many more [1,2]. But quality issues in terms of reproducibility and functionality still limit the potential of AM for many industrial applications. Due to the fact that supervised neural networks need the input values (process parameters) as well as the output values (quality characteristics), prediction is also possible in both directions. This opens up great opportunities for AM and HIP projects. Quality or process parameter prediction paves the way for overcoming existing quality constraints or long development times and enables for challenging industrial applications. Furthermore, quality is not an absolute value, which means it should always be defined relatively to the intended use. Quality must be set according to the required functionality. The developed prediction models can be used to make AM and HIP more flexible for customised projects, reducing costs and time to market.

Further research should extend the existing models with a larger number of parameter variations, as well as other important influencing factors (powder characteristics, other materials and manufacturing technologies, as well as more human or process related influences). A larger amount of data and more trained influences will lead to a better generalisation of the models and reduce incorrect predictions.

10. References

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Appendix

A.1. Publications

Publication I:

A Novel Classification Method for Pores in Laser Powder Bed Fusion
(Nudelis et al. [16])

Publication II:

Defect-based Analysis of the Laser Powder Bed Fusion Process using X-Ray
Data
(Nudelis et al. [17])

Publication III:

Pore Tracing in Additive Manufactured and Hot Isostatic Pressed Components
(Nudelis et al. [18])

A.2. Original Data from PBF-LB/M Process

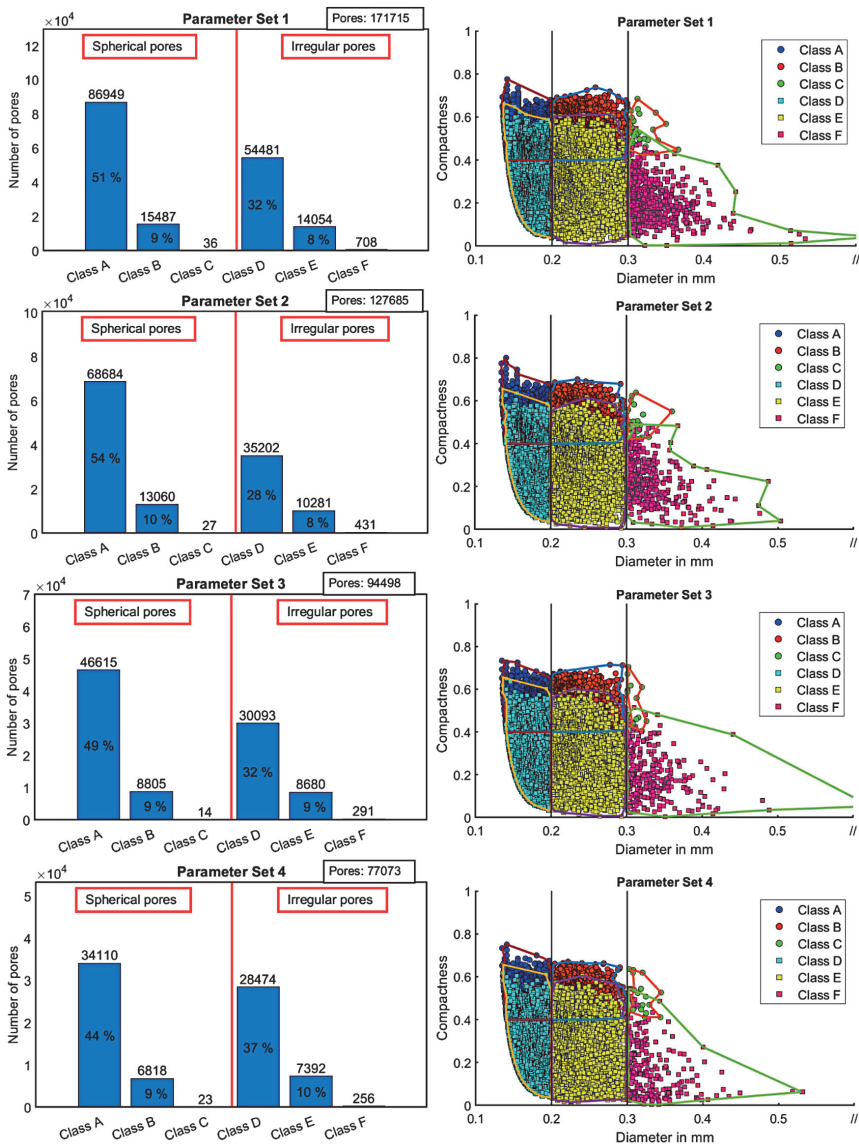


Figure 45: Original pore data for PBF-LB/M (Parameter Set 1–4)

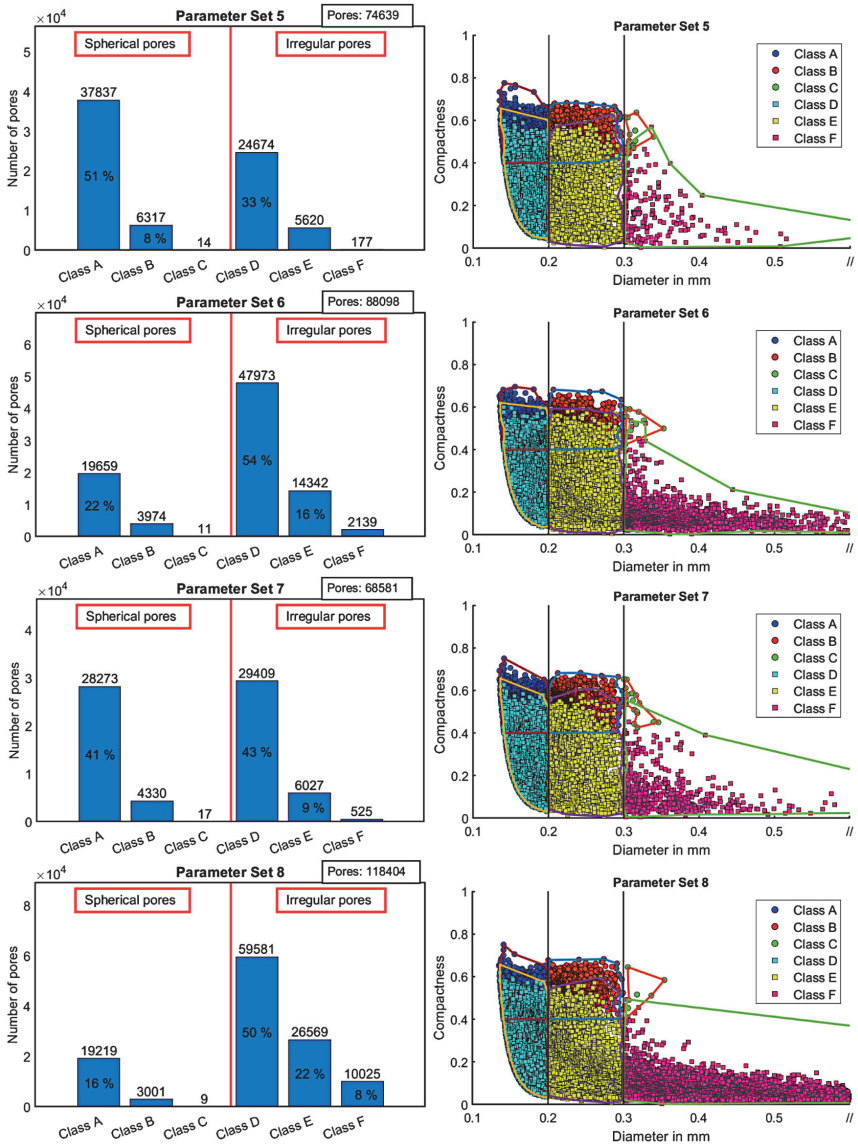


Figure 46: Original pore data for PBF-LB/M (Parameter Set 5–8)

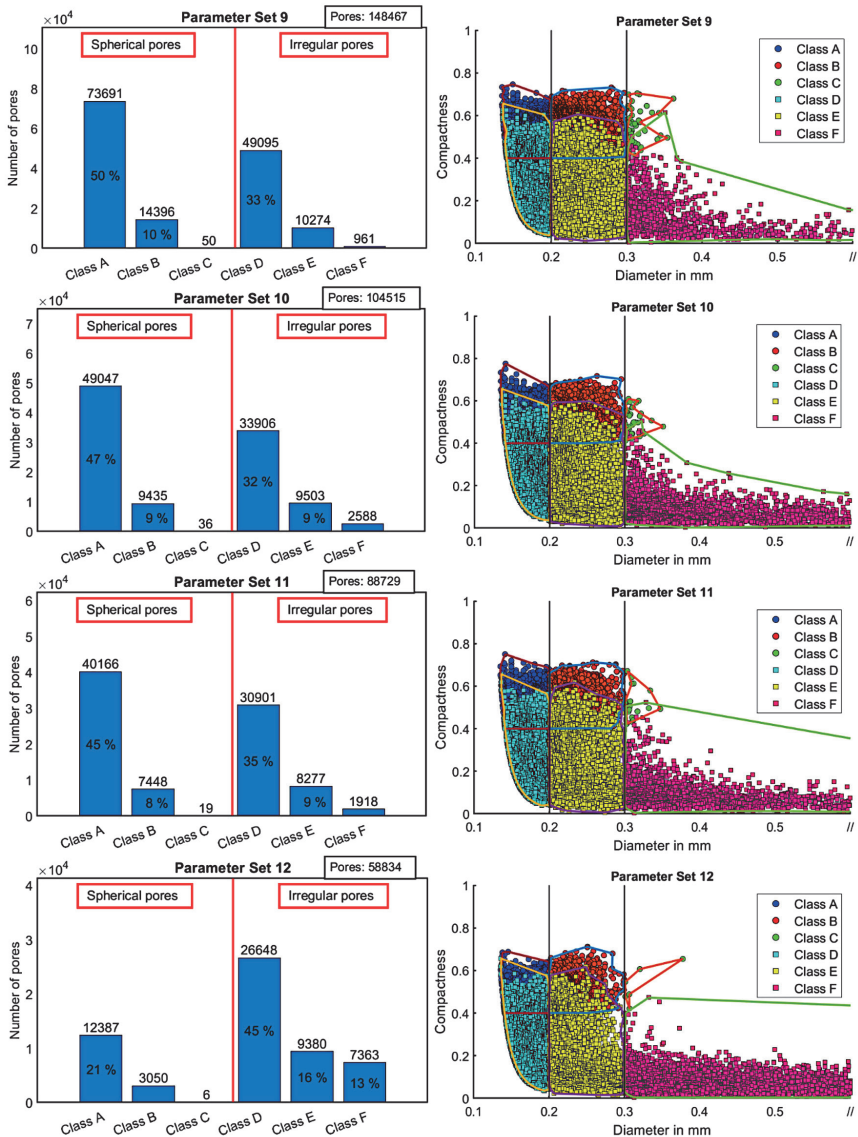


Figure 47: Original pore data for PBF-LB/M (Parameter Set 9–12)

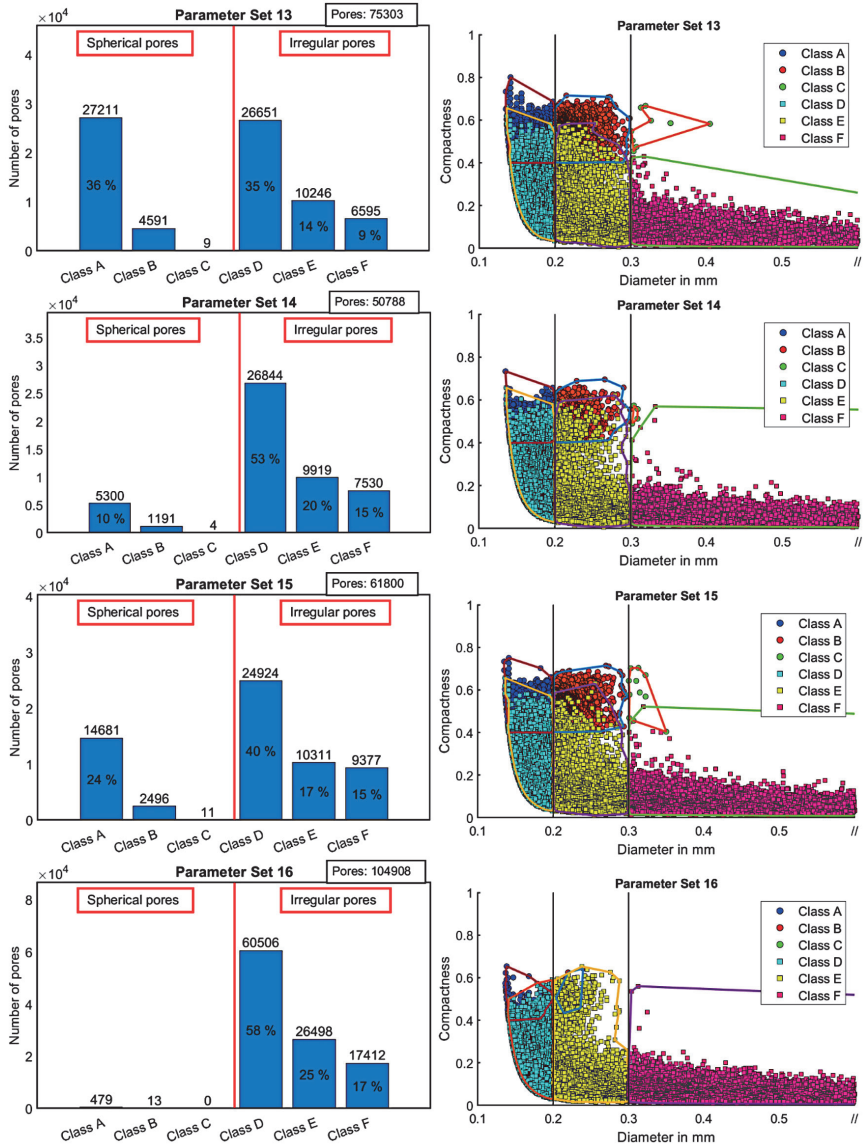


Figure 48: Original pore data for PBF-LB/M (Parameter Set 13–16)

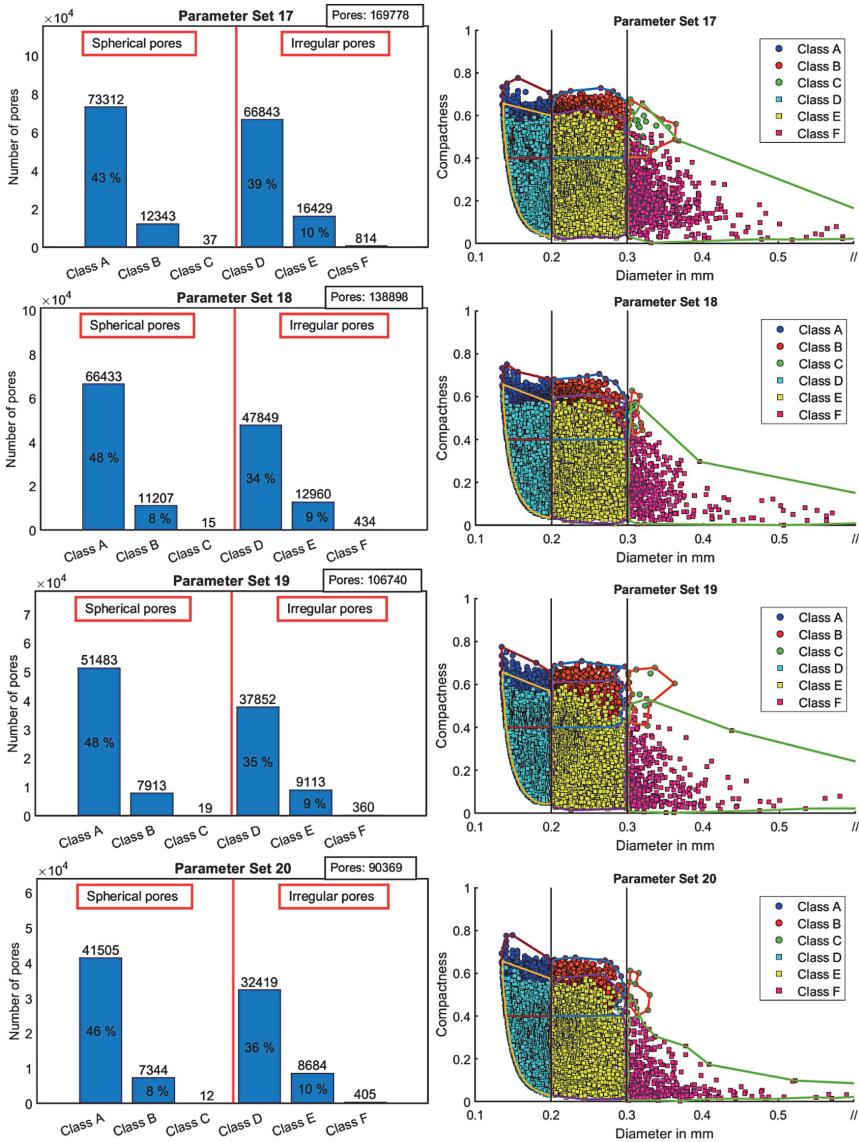


Figure 49: Original pore data for PBF-LB/M (Parameter Set 17–20)

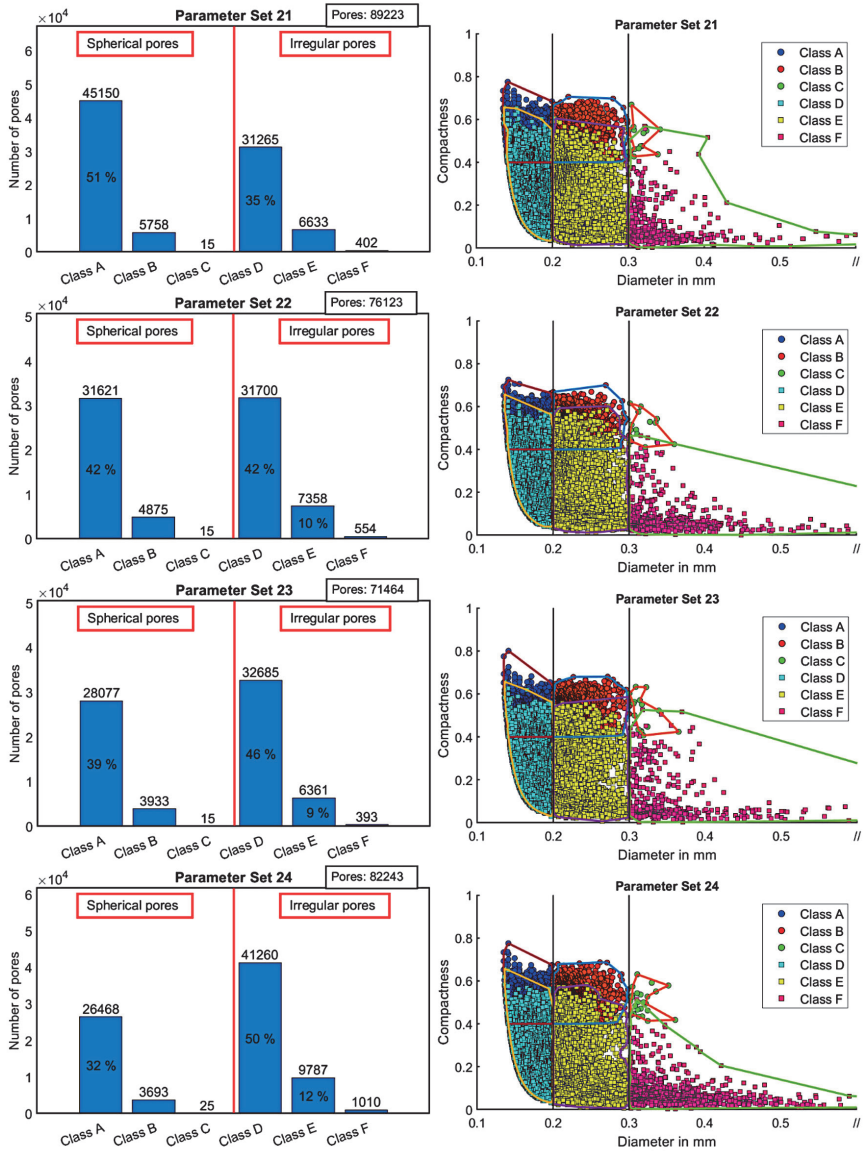


Figure 50: Original pore data for PBF-LB/M (Parameter Set 21–24)

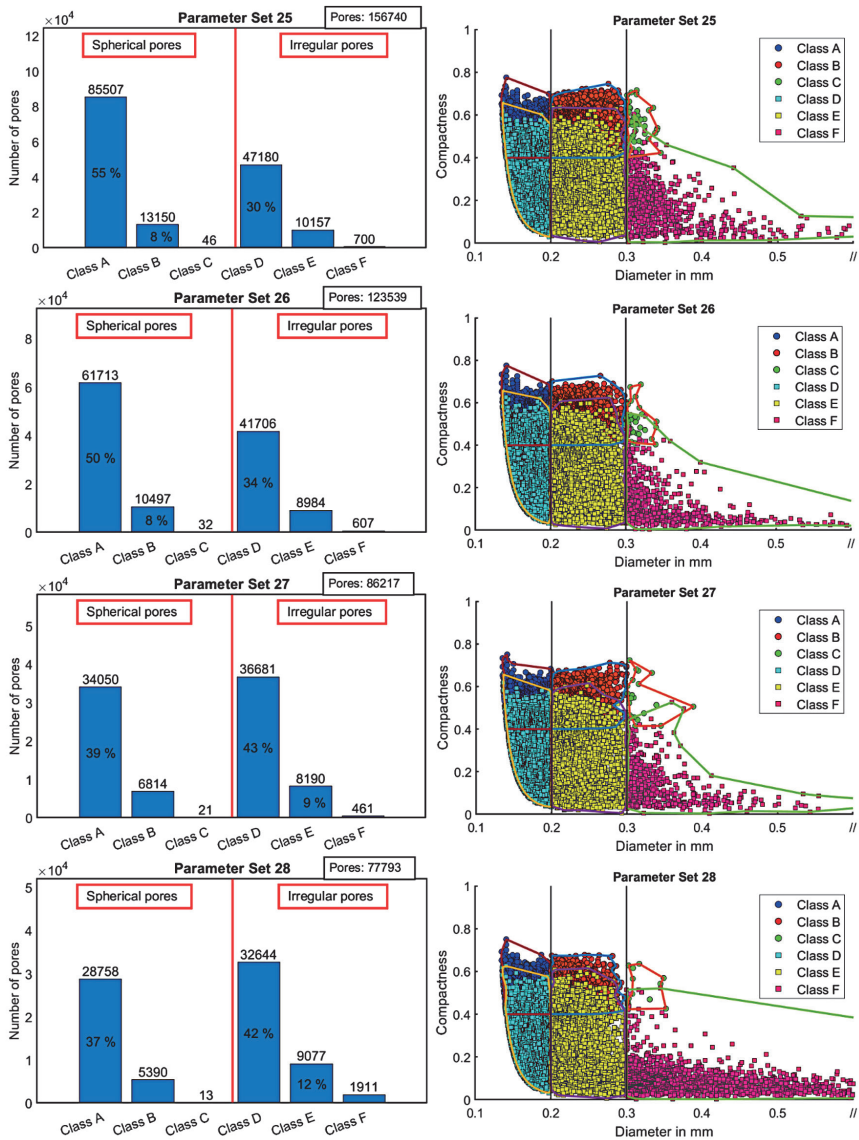


Figure 51: Original pore data for PBF-LB/M (Parameter Set 25–28)

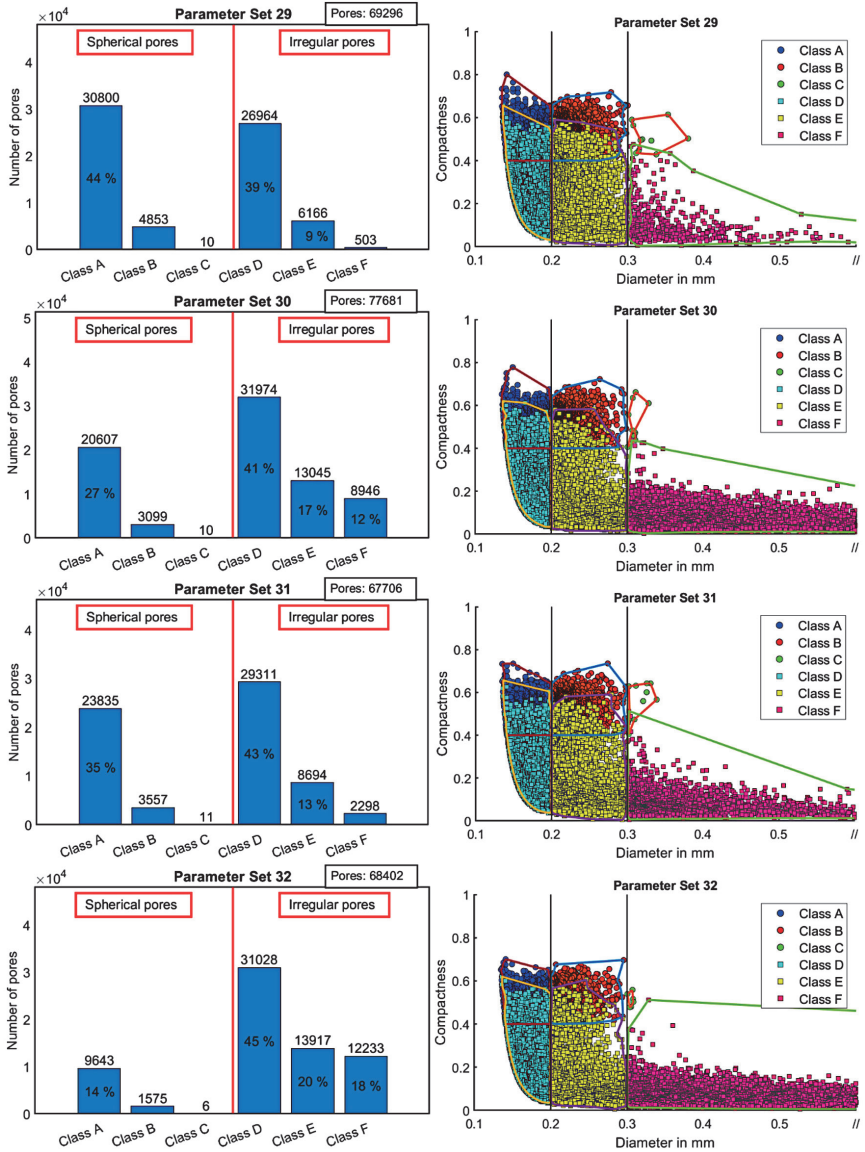


Figure 52: Original pore data for PBF-LB/M (Parameter Set 29–32)

A.3. Original Data from HIP Process

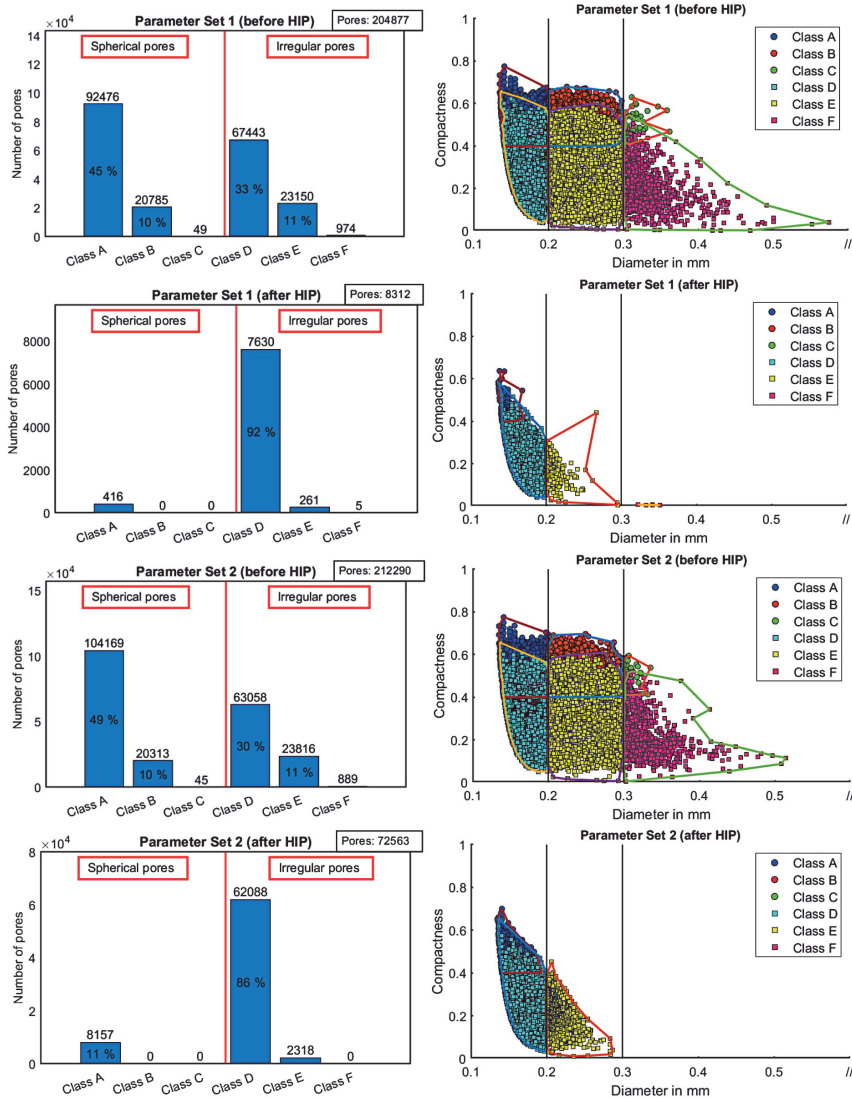


Figure 53: Original pore data for HIP (Parameter Set 1–2)

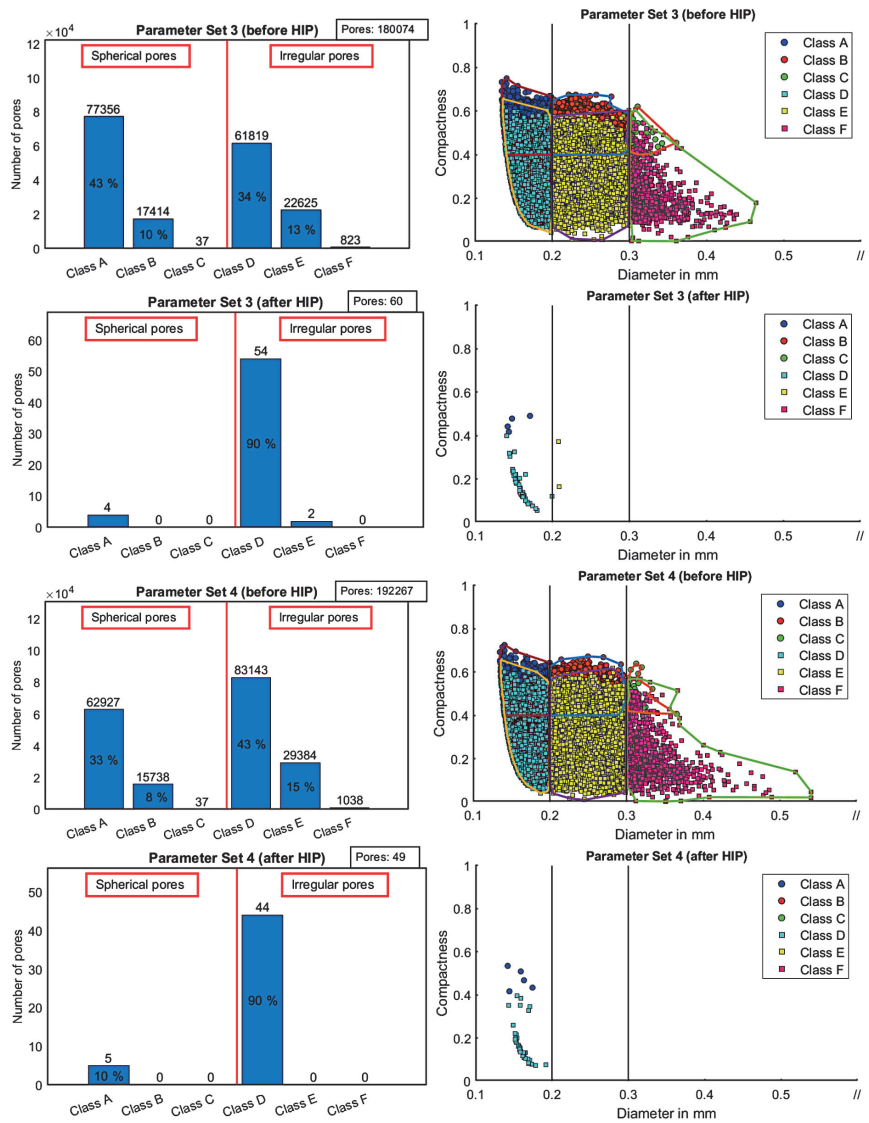


Figure 54: Original pore data for HIP (Parameter Set 3–4)

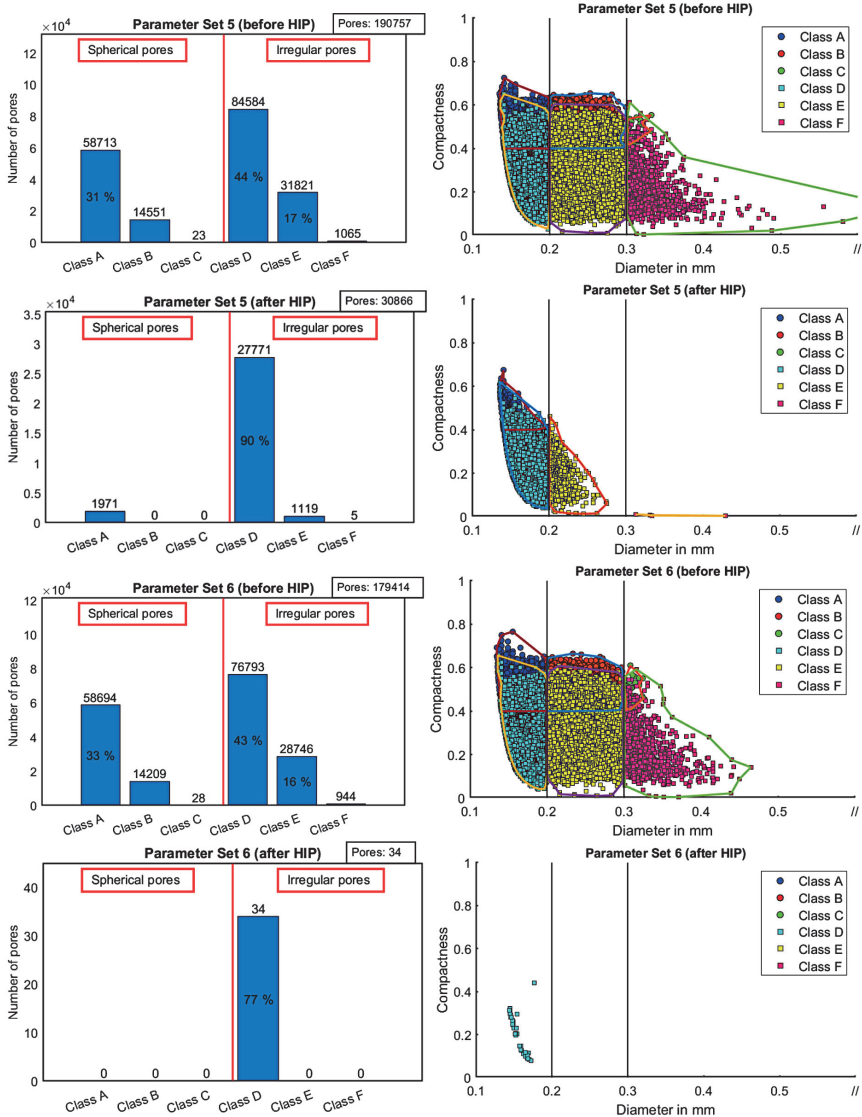


Figure 55: Original pore data for HIP (Parameter Set 5–6)

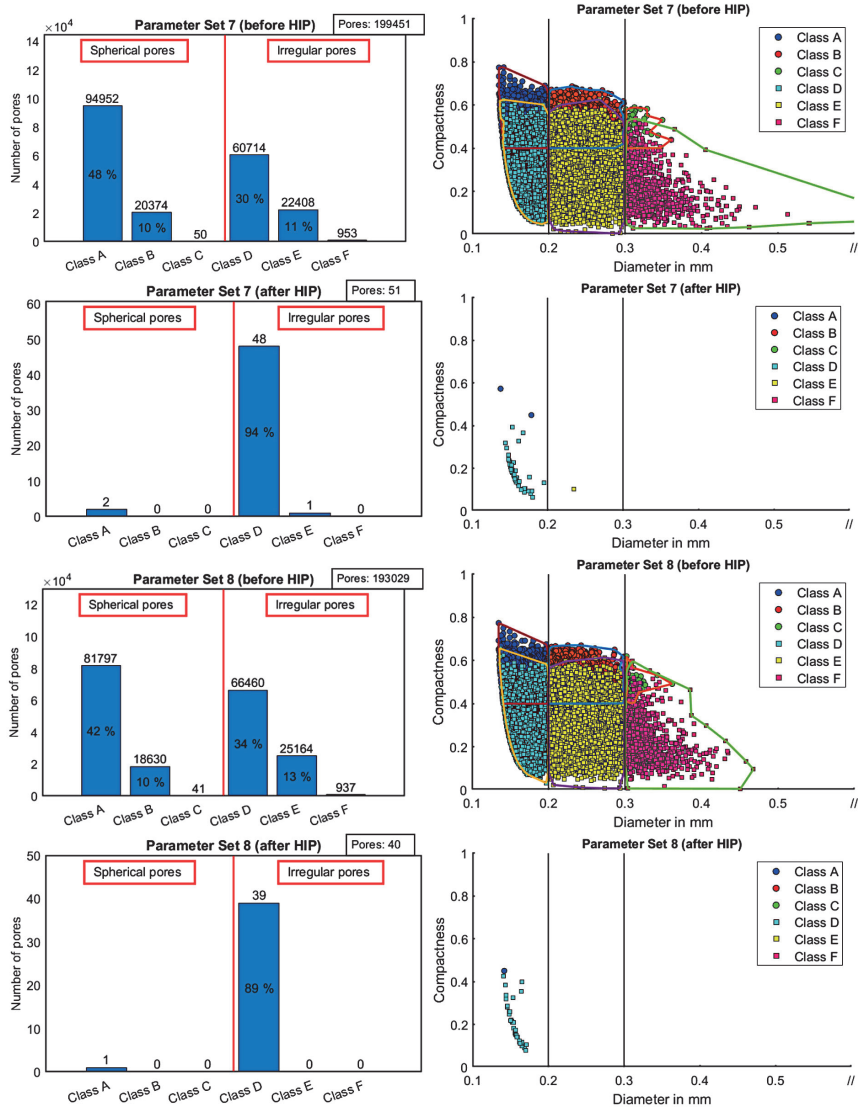


Figure 56: Original pore data for HIP (Parameter Set 7–8)

A.4. Separated ANN Model for Pore Types (PBF-LB/M)

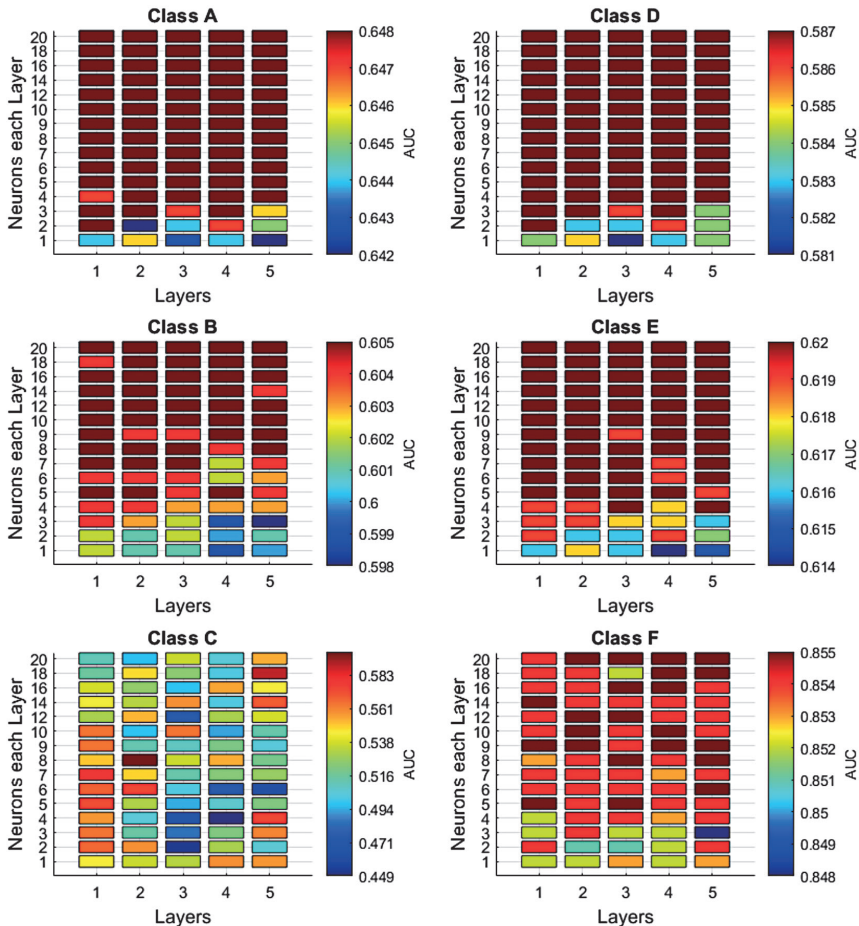


Figure 57: AUC for pore classes A–F in different separated neural networks (for PBF-LB/M pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

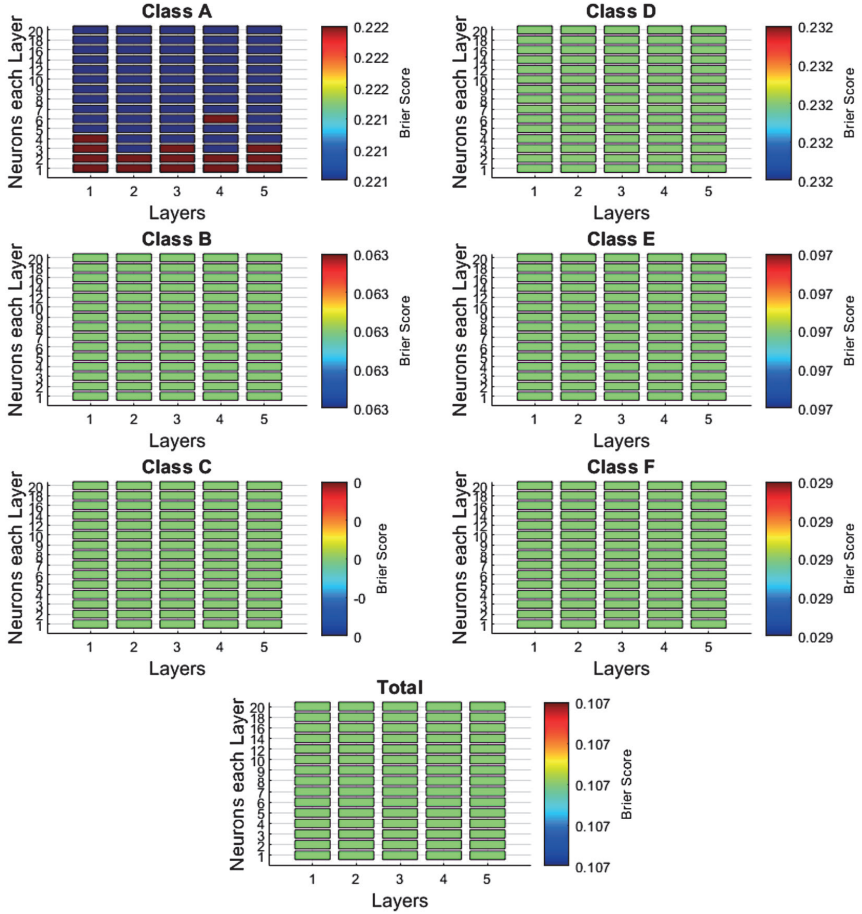


Figure 58: Brier-score for pore classes A–F and the total Brier-score in different separated neural networks (for PBF-LB/M pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

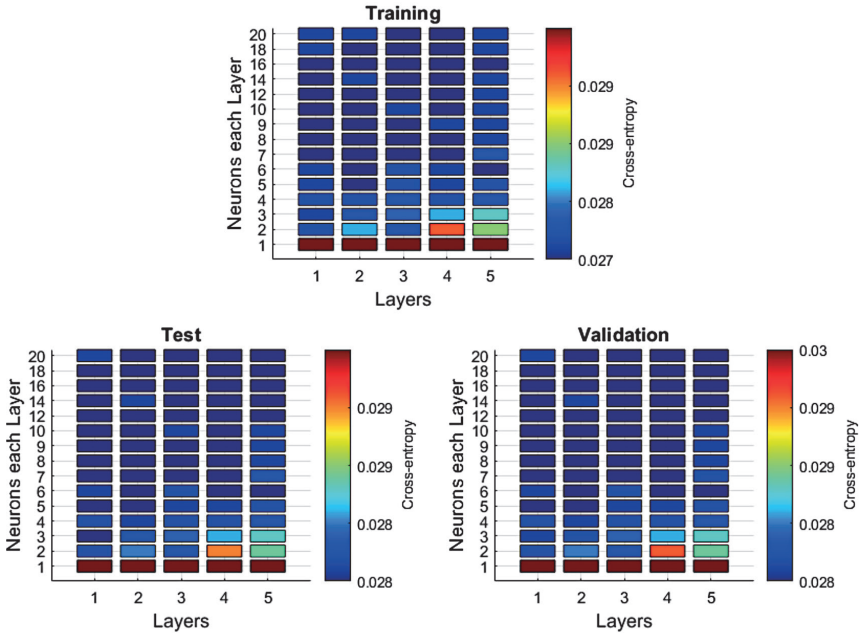


Figure 59: Cross-entropy for the training, test and validation data set in different separated neural networks (for PBF-LB/M pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

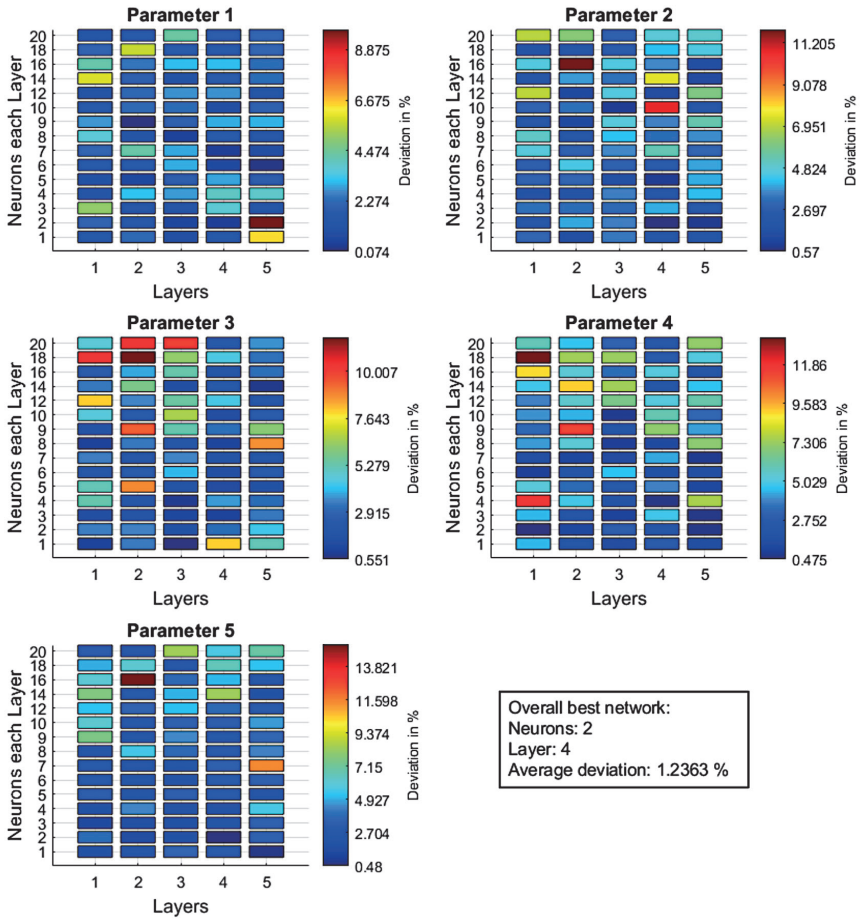


Figure 60: Additional generalisation test on unknown data for the PBF-LB/M pore class prediction. 5 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained separated neural networks with different numbers of hidden layers and neurons in each hidden layer

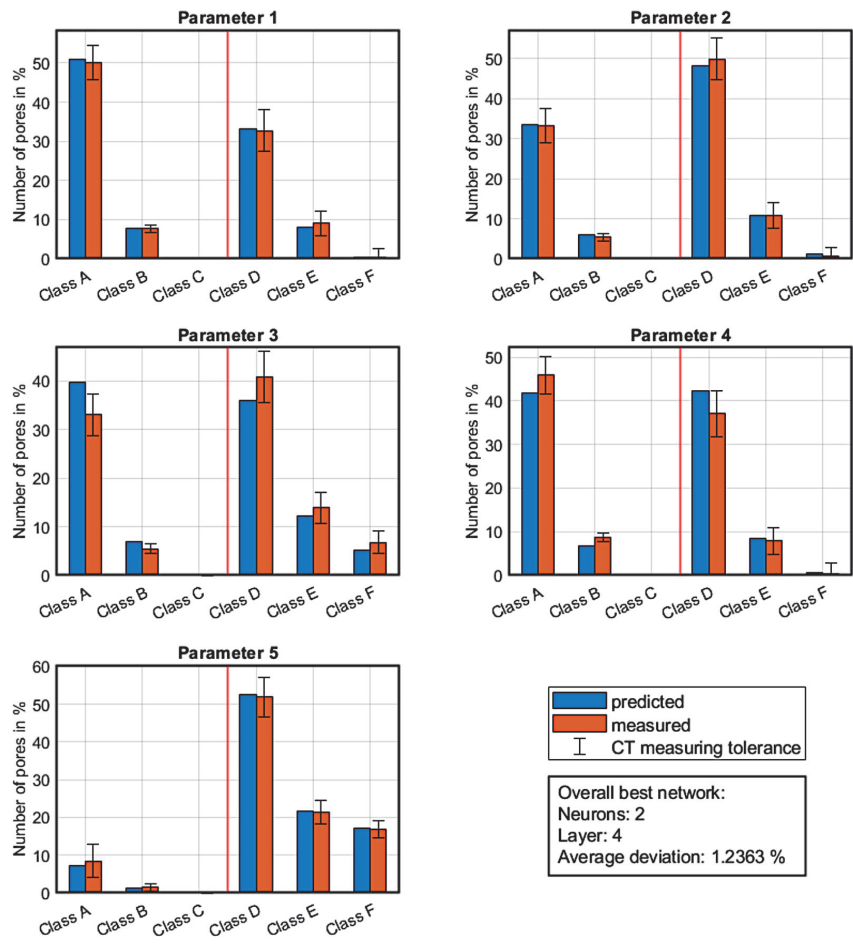


Figure 61: Illustration of the PBF-LB/M pore class prediction results of the best separated network using the example of 5 unknown parameter data sets (additional testing)

A.5. Fully Connected ANN Model for Part Density (PBF-LB/M)

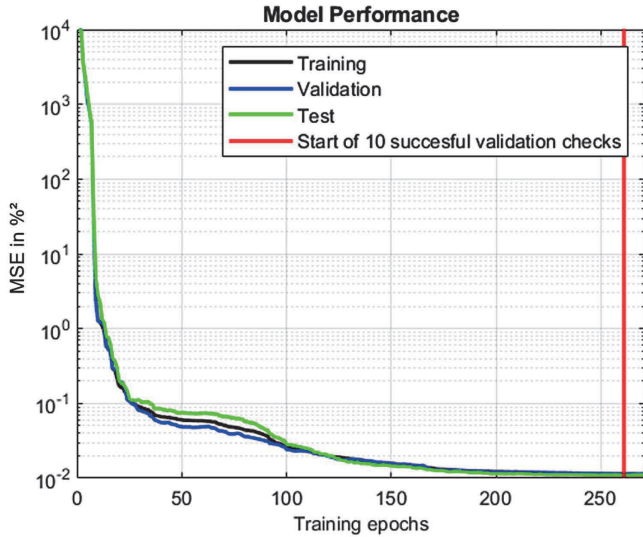


Figure 62: Model performance of the best fully connected network for PBF-LB/M part density prediction (best network: 2 hidden layers and 9 neurons per layer)

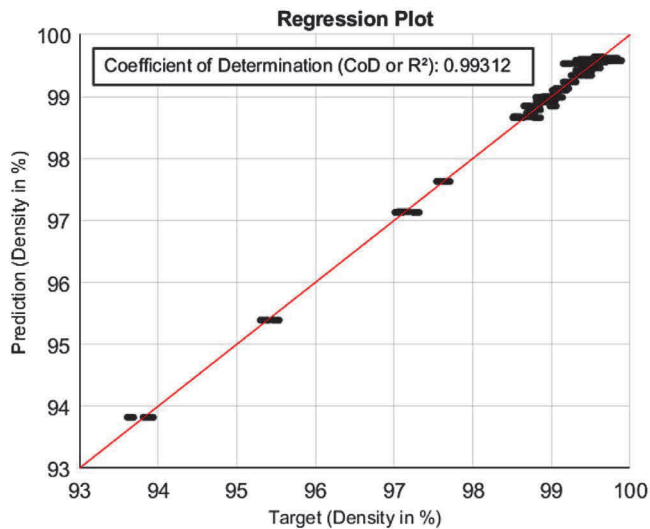


Figure 63: Regression plot of the best fully connected network for PBF-LB/M part density prediction (best network: 2 hidden layers and 9 neurons per layer)

A.6. Separated ANN Model for Pore Types (HIP)

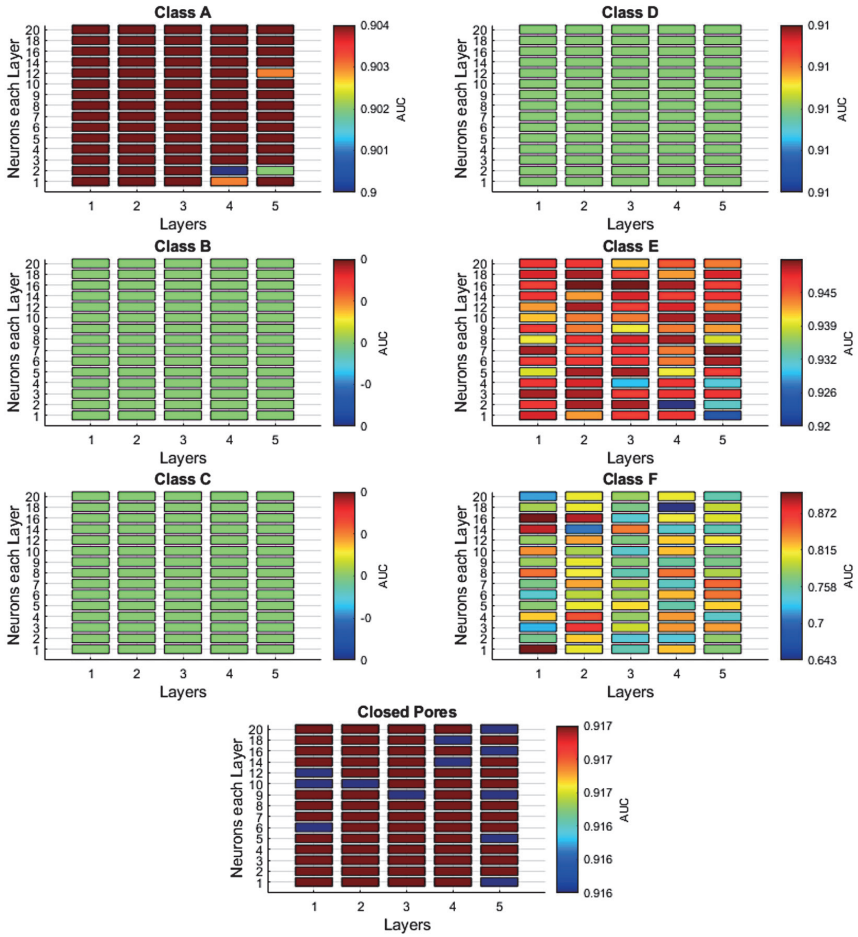


Figure 64: AUC for pore classes A–F and closed pores in different separated neural networks (for HIP prediction) with different numbers of hidden layers and neurons in each hidden layer

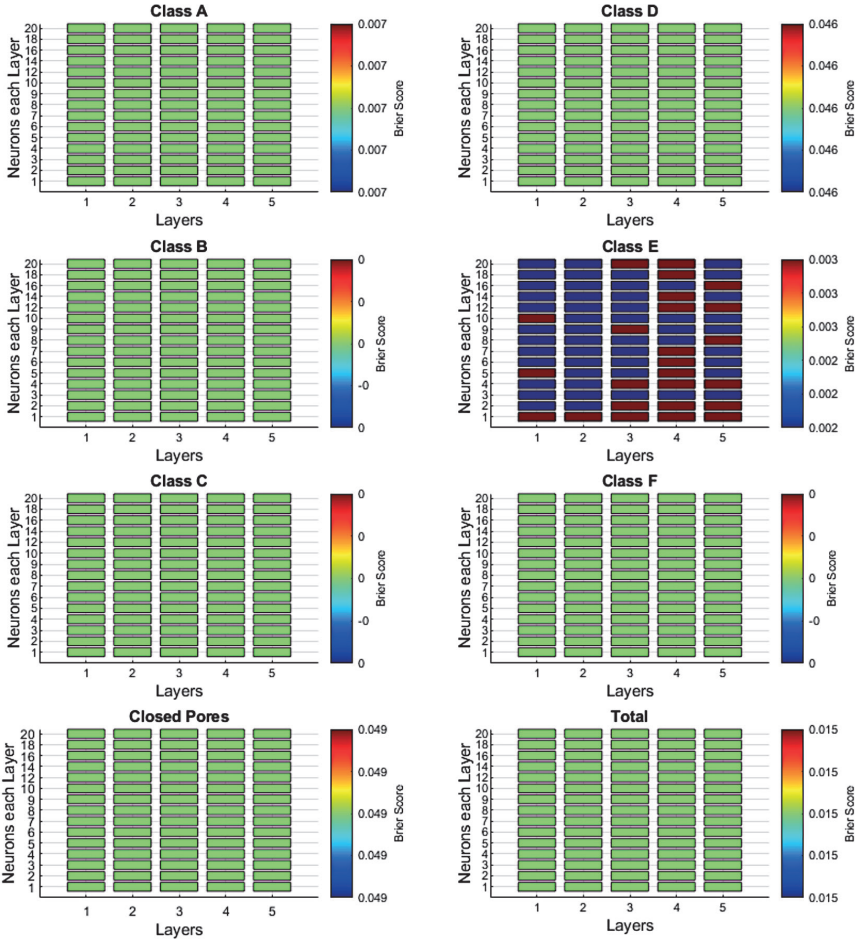


Figure 65: Brier-score for pore classes A–F as well as closed pores and the total Brier-score in different separated neural networks (for HIP prediction) with different numbers of hidden layers and neurons in each hidden layer

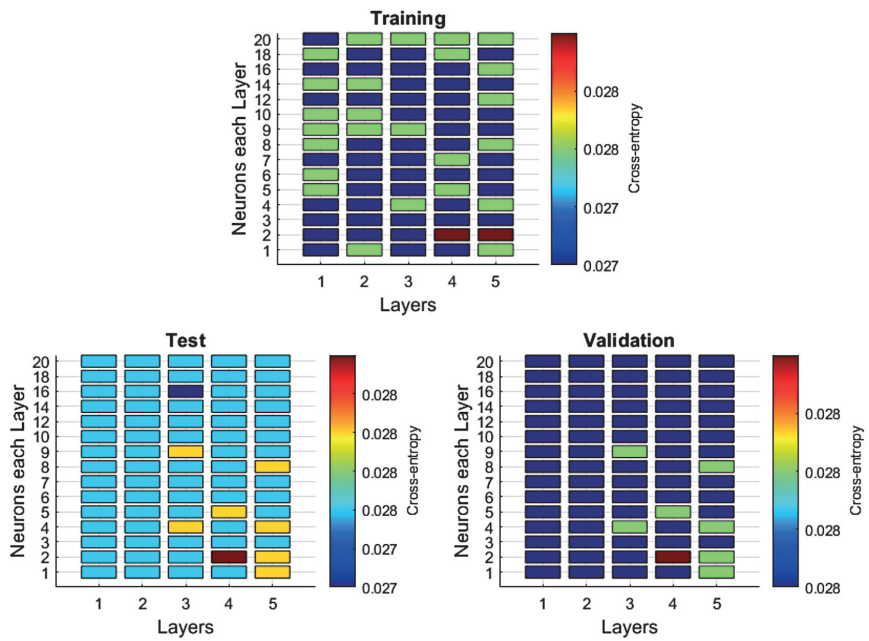


Figure 66: Cross-entropy for the training, test and validation data set in different separated neural networks (for HIP pore class prediction) with different numbers of hidden layers and neurons in each hidden layer

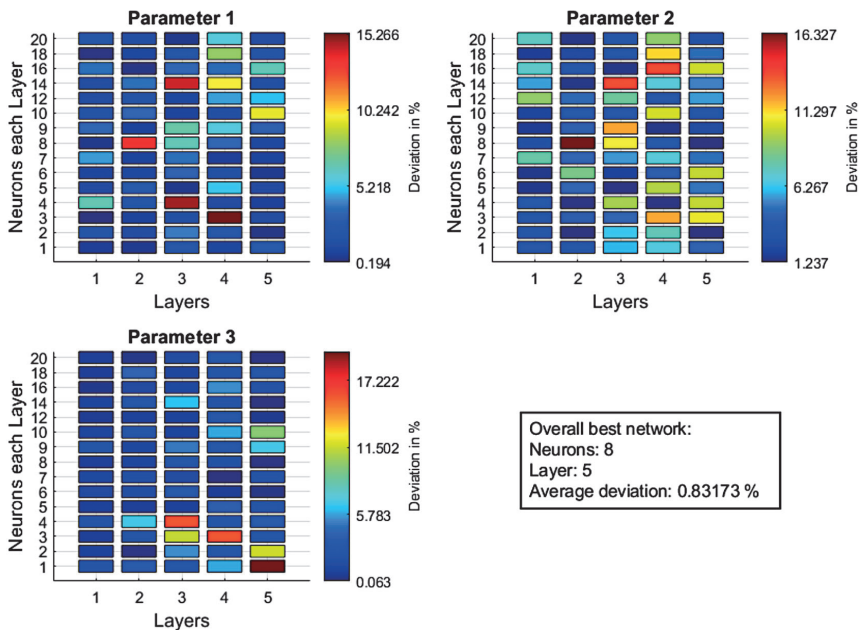


Figure 67: Additional generalisation test on unknown data for the HIP pore class prediction. 3 unknown parameter data sets compared with the ML prediction. Deviations for each test parameter set in different trained separated neural networks with different numbers of hidden layers and neurons in each hidden layer

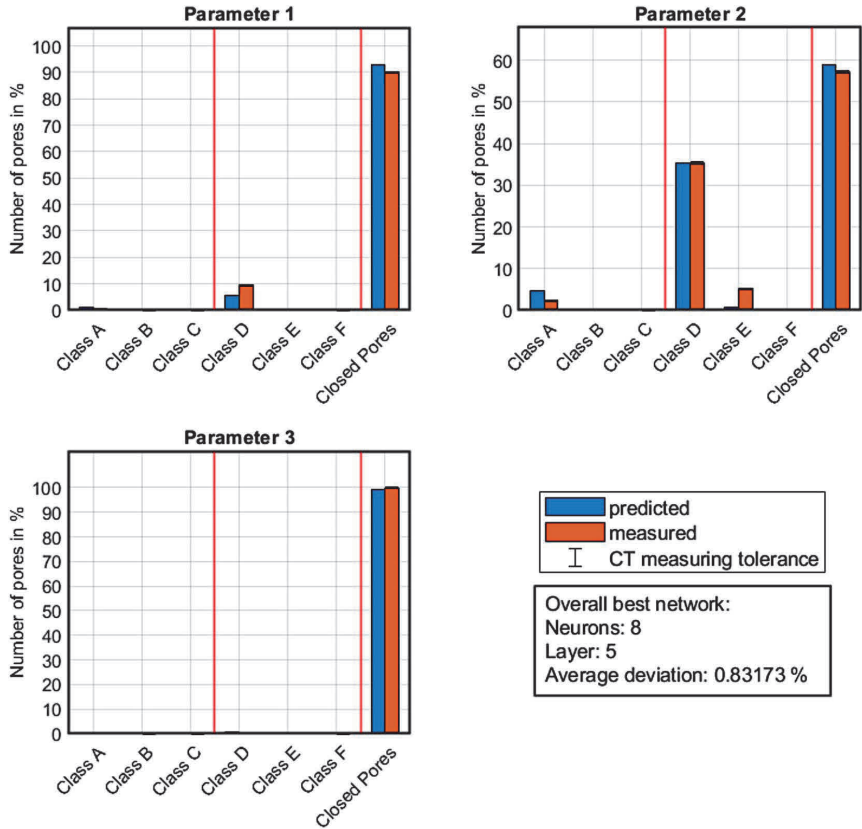


Figure 68: Illustration of the HIP pore class prediction results of the best separated network using the example of 3 unknown parameter data sets (additional testing)

A.7. Fully Connected ANN Model for Hardness (HIP)

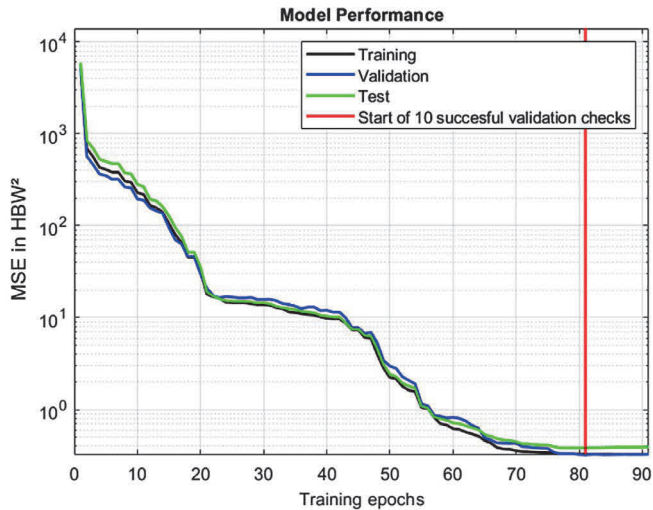


Figure 69: Model performance of the best fully connected network for HIP hardness prediction (best network: 4 hidden layers and 18 neurons per layer)

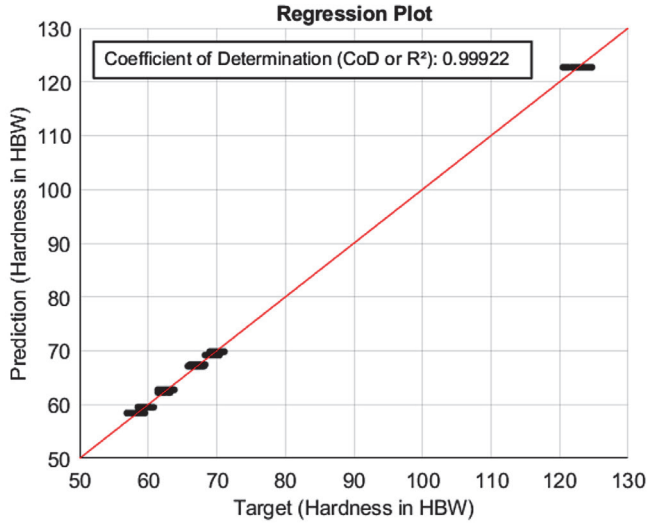


Figure 70: Regression plot of the best fully connected network for HIP hardness prediction (best network: 4 hidden layers and 18 neurons per layer)

Additive manufacturing (AM) using laser powder bed fusion (PBF-LB/M) has many advantages such as design freedom and sustainability. However, AM also suffers from internal defects that limit its functionality. Furthermore, post-treatment methods like hot isostatic pressing (HIP) promise to enhance material properties. This work aims to develop a machine learning model using artificial neural networks, to predict PBF-LB/M or HIP process parameters based on quality characteristics.