## INSTITUTO TECNOLÓGICO DE AERONÁUTICA



#### Gabriel Barbosa Martinz

# USE OF GENERATIVE NEURAL NETWORKS FOR INSTANCE SPACE CODIFICATION AND GENERATION OF DATA WITH SPECIFIC PROPERTIES

Final Paper 2023

**Course of Computer Engineering** 

#### Gabriel Barbosa Martinz

# USE OF GENERATIVE NEURAL NETWORKS FOR INSTANCE SPACE CODIFICATION AND GENERATION OF DATA WITH SPECIFIC PROPERTIES

#### Advisor

Prof<sup>a</sup>. Dr<sup>a</sup>. Ana Carolina Lorena (ITA)

#### COMPUTER ENGINEERING

São José dos Campos Instituto Tecnológico de Aeronáutica

#### Cataloging-in Publication Data

#### **Documentation and Information Division**

Barbosa Martinz, Gabriel

Use of generative neural networks for instance space codification and generation of data with specific properties / Gabriel Barbosa Martinz.

São José dos Campos, 2023.

31f

Final paper (Undergraduation study) – Course of Computer Engineering– Instituto Tecnológico de Aeronáutica, 2023. Advisor: Prof<sup>a</sup>. Dr<sup>a</sup>. Ana Carolina Lorena.

1. Neural networks. 2. Instance space. 3. GAN. I. Instituto Tecnológico de Aeronáutica. II. Title.

#### BIBLIOGRAPHIC REFERENCE

BARBOSA MARTINZ, Gabriel. Use of generative neural networks for instance space codification and generation of data with specific properties. 2023. 31f. Final paper (Undergraduation study) – Instituto Tecnológico de Aeronáutica, São José dos Campos.

#### **CESSION OF RIGHTS**

AUTHOR'S NAME: Gabriel Barbosa Martinz

PUBLICATION TITLE: Use of generative neural networks for instance space codification

and generation of data with specific properties.

PUBLICATION KIND/YEAR: Final paper (Undergraduation study) / 2023

It is granted to Instituto Tecnológico de Aeronáutica permission to reproduce copies of this final paper and to only loan or to sell copies for academic and scientific purposes. The author reserves other publication rights and no part of this final paper can be reproduced without the authorization of the author.

Gabriel Barbosa Martinz Rua H8B, 203 12.228-461 – São José dos Campos–SP

# USE OF GENERATIVE NEURAL NETWORKS FOR INSTANCE SPACE CODIFICATION AND GENERATION OF DATA WITH SPECIFIC PROPERTIES

This pu	blication	was ac	cepted	like I	Final	Work	of Und	ergradı	ation	Study
•			Gabri	el Bai	rbosa	Marti	nz			
					thor					
				Au	tillor					
			Ana Ca	arolina	a Lor	ena (I'	ΓΑ)			
				$\operatorname{Ad}$	visor					

Prof. Dr. Marcos Máximo Course Coordinator of Computer Engineering

Aos amigos da Graduação do ITA por motivarem tanto a criação deste template pelo Fábio Fagundes Silveira quanto por motivarem a mim e outras pessoas a atualizarem e aprimorarem este excelente trabalho.

# Acknowledgments

Primeiramente, gostaria de agradecer ao Dr. Donald E. Knuth, por ter desenvolvido o T<sub>F</sub>X.

Ao Dr. Leslie Lamport, por ter criado o LATEX, facilitando muito a utilização do TEX, e assim, eu não ter que usar o Word.

Ao Prof. Dr. Meu Orientador, pela orientação e confiança depositada na realização deste trabalho.

Ao Dr. Nelson D'Ávilla, por emprestar seu nome a essa importante via de trânsito na cidade de São José dos Campos.

Ah, já estava esquecendo... agradeço também, mais uma vez ao TEX, por ele não possuir vírus de macro :-)

## **Abstract**

One topic of study in Machine Learning is the study of algorithmic performance and which methodologies may be used to assess this performance. A methodology known as Instance Space Analysis has been used to relate predictive performance in classification algorithms to instance hardness (how hard an instance is for an algorithm to classify). The original methodology has been defined with the instance being an entire dataset, but further work has been made to make the instance as fine-grained as an individual observation. In this work we will build upon this methodology and we propose the creation of a generative neural network model to generate new observations for a classification algorithm with predefined hardness properties.

# List of Figures

FIGURE 2.1 –	Model of an artificial neuron	15
FIGURE 2.2 –	A model of a simple fully-connected neural network with 3 inputs,	
	3 outputs and a hidden layer with 4 nodes	16
FIGURE 2.3 –	Flowchart of the GAN training model	17
FIGURE 3.1 –	ISA framework. Extracted from (MUÑOZ et al., 2018). The ASP is highlighted in blue	20
FIGURE 3.2 –	ISA framework for a single dataset. Extracted from (PAIVA et al., 2022)	22

# List of Tables

TABLE 3.1 –	Hardness measures	used in (PAI	VA et al., 2022)			24
-------------	-------------------	--------------	------------------	--	--	----

# Contents

1	Int	ROI	DUCTION	12
	1.1	Mot	tivation	12
	1.2	Obj	ective	13
	1.3	Sco	pe	13
	1.4	Out	line of this work	13
2	Ma	CHI	ne Learning	14
	2.1	Clas	ssification	14
	2.2	Neu	ıral networks	14
	2.2	2.1	Artificial neuron	15
	2.2	2.2	The network	15
	2.2	2.3	Learning	16
	2.3	Ger	nerative Adversarial Networks	17
3	Ins	TAN	CE SPACE ANALYSIS	19
	3.1	Inst	ance spaces	19
	3.1	.1	Instance Space construction	21
	3.1	.2	Footprint analysis	22
	3.2	ISA	for a single dataset	22
	3.2	2.1	Hardness measures	23
	3.2	2.2	Performance assessment	24
	3.2	2.3	Feature selection	24
	3.2	2.4	IS representation and footprints	25

CONTENTS	xi

4	ME	THODOLOGY	26
	4.1	Instance Space generation	26
	4.2	Generator and Discriminator creation	26
	4.3	Re-evaluation of the generated data	26
5	RE	SULTS	28
	5.1	Planned results	28
6	Со	NCLUSION	29
	6.1	Preliminary conclusions and future work	29
	6.2	Work plan	29
В	IBLIC	OGRAPHY	30
A	PPEN	IDIX A – INSTANCE HARDNESS	31
	<b>A.1</b>	Metrics used in subsection 3.2.1	31

## 1 Introduction

#### 1.1 Motivation

Often in a problem being tackled with Machine Learning (ML) techniques one of the most important part of the solving process is the algorithm selection. Each algorithm has a specific bias which makes it more suitable for some classes of problems than others (PAIVA et al., 2022).

It is desirable, then, that we may have a way of measuring the relationship of the performance of a given algorithm in a problem with the problem's characteristics, since knowing which data is easy or difficult for a given model to classify is useful in the way that we may make changes to the original model.

(Muñoz et al., 2018) has introduced a methodology called Instance Space Analysis (ISA), a novel way of performance evaluation and algorithm selection in classifiers by mapping the statistical properties of an instance (an entire dataset) into how difficult the instance is for the classification algorithm to perform. Further, in (PAIVA et al., 2022), the methodology has been modified to have a more fine-grained analysis, with the instance being reduced to an individual observation in a classification dataset.

Given this, we can map each observation into a hardness level. One type of model that may give us new information from this data is a Generative Adversarial Network (GAN) architecture as defined by (GOODFELLOW et al., 2014). This architecture is based on a zero-sum game, with a generator network trying to create data matching the original data and a discriminator network trying to discern between the original data and the generated data.

Using this, we can use the trained generator to create data with specific hardness levels and set a difficulty of classification for an entire dataset. We can use this to verify how the original model behaves with data with a given difficulty profile or to challenge the model.

## 1.2 Objective

This work's objective lies in providing a framework for data generation based on the relationship between instance hardness and classification performance using the GAN architecture and monitor the original model's behaviour using the generated data.

## 1.3 Scope

The scope of this work will be limited to exploring a GAN implementation for the generation of data, creating a Generator and a Discriminator. The modelling will be made entirely using Python, with the PyTorch (PASZKE et al., 2019) framework. PyHard (PAIVA et al., 2022) will be used for reproducing the ISA methodology.

### 1.4 Outline of this work

# 2 Machine Learning

This chapter will introduce Machine Learning (ML) concepts and techniques being explored in this work, namely the classification problem, neural networks and the Generative Adversarial Network architecture.

#### 2.1 Classification

In Statistics and Machine Learning, a problem is defined as a classification problem when it consists in identifying to which categories a member of a population belongs to. An example might be identifying which race of domestic cat is shown in a picture containing a cat. An algorithm that implements classification is known as a classifier. The classifier works by analysing each observation into dependent variables and either mapping those to the categories or by comparing each observation to previous observations by means of a similarity function or loss function.

Terminology between Statistics and Machine Learning tend to differ. In this work, we will be using the terminology found in Machine Learning, namely:

- dependent variables are called features;
- categories are called classes;

In this work, we will not focus on a specific classification algorithm since ISA is not dependent on the algorithm used, only on the problem of classification.

#### 2.2 Neural networks

Neural networks, formally called artificial neural networks (ANNs), are computational models inspired by networks of biological neurons (PURI et al., 2016). They are made up of multiple nodes called artificial neurons that map an input to an output based on mathematical operations. This model is used extensively in ML applications because of its perceived intelligent behaviour that come from the interactions between neurons.

#### 2.2.1 Artificial neuron

The artificial neuron is the most basic block of an ANN. It maps inputs to an output in the given fashion:

$$y = f(\mathbf{w} \cdot \mathbf{x} + b),\tag{2.1}$$

where the symbols are defined as:

$$\mathbf{x} = [x_1, x_2, \dots, x_n]$$
 Input vector;  
 $\mathbf{w} = [w_1, w_2, \dots, w_n]$  Weight vector;  
 $f$  Activation function;  
 $y$  Neuron output. (2.2)

Figure 2.1 shows the artificial neuron model. This model of neuron is useful because it incorporates both the linear combination of input values and bias and the non-linearity of the activation function, which means it may function as a part of an universal function approximator (HORNIK *et al.*, 1989).

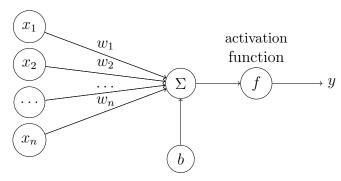


FIGURE 2.1 – Model of an artificial neuron.

#### 2.2.2 The network

As said before, an ANN is a network of artificial neurons. Such network may be built by having the neurons configured in layers, having each neuron in a layer connected only to neurons in either preceding or following layers or with other arrangement of connections. Figure 2.2 shows a simple model of a fully-connected (a neuron in a layer connects to every neuron in the next layer) neural network, having 3 inputs, 4 middle nodes (called a hidden layer) and 3 output nodes.

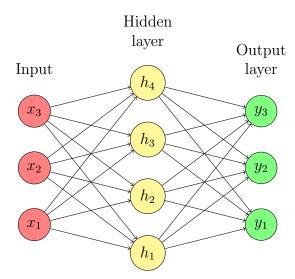


FIGURE 2.2 – A model of a simple fully-connected neural network with 3 inputs, 3 outputs and a hidden layer with 4 nodes.

#### 2.2.3 Learning

Learning is the process by which an ANN adapts itself to a given task using data. It involves adjusting the weights of the network to improve some predefined metric (e.g. accuracy) and minimizing observed errors. In practice, learning is done by defining a loss function which is evaluated during learning and as long as its output (called loss, for short) decreases, the learning continues.

Most learning models are applications of optimization theory, like the gradient descent algorithm. In this algorithm the purpose is to find a local minima by moving against the gradient of the function. It is the basis for the Adam optimizer (KINGMA; BA, 2017), used extensively in ANNs.

#### 2.2.3.1 Learning rate

The learning rate is a parameter in an optimization algorithm, defining the size of each step towards the local minima of a loss function. Higher learning rates shorten the learning time, but at a cost of possibly never converging and higher errors, while setting it at a value too low might have it converging in an undesirable local minimum.

#### 2.2.3.2 Backpropagation

Backpropagation is a method to adjust the weights of the network and minimize the mean squared error. It computes the gradient of the loss function with respects to the weights and propagates backwards from the output layer to avoid redundant calculations.

#### 2.3 Generative Adversarial Networks

A Generative Adversarial Network (GAN) is an architecture for estimating generative artificial intelligence models. It consists of a two-player minimax game between two ANNs: a generative model G and a discriminative model D. The purpose of D is to estimate the probability that a sample came from the training data instead of coming from G, and the purpose of G is to minimize that probability. A unique solution exists where D outputs the probability of  $\frac{1}{2}$  everywhere (GOODFELLOW et al., 2014). The generator G is, then, not trained to minimize a loss function, but to fool the discriminator D.

We will now be defining some notation for more formal modelling. Let  $\mathbf{x}$  be the input data,  $D(\mathbf{x})$  is then the output of the discriminator over the training data, which is the probability that the input data came from the training data rather than the generator. For the generator, let  $\mathbf{z}$  be a latent space vector sampled from a standard normal distribution.  $G(\mathbf{z})$  represents the generator's output, mapping  $\mathbf{z}$  to the data space.

 $D(G(\mathbf{z}))$  is therefore the probability that a generated input came from the training data. The goal of G is to estimate the distribution which the training data comes from  $(p_{data})$  so that it may draw samples from this estimation  $(p_G)$  (GOODFELLOW *et al.*, 2014). The minimax loss function will be, therefore:

$$\min_{G} \max_{D} V(D, G) = \mathbb{E}_{\mathbf{x} \sim p_{data}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})}[\log(1 - D(G(\mathbf{z})))]$$
(2.3)

In theory, the solution of this game will be when  $p_G = p_{data}$  and the discriminator will guess every generated input randomly  $(D(G(\mathbf{z})) = \frac{1}{2})$ . Figure 2.3 shows a flowchart of this training model. Algorithm 1 is the training algorithm defined in (GOODFELLOW *et al.*, 2014).

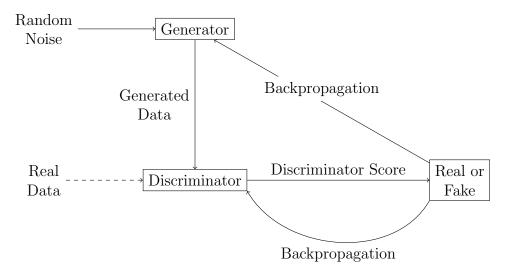


FIGURE 2.3 – Flowchart of the GAN training model.

**Algorithm 1:** Minibatch stochastic gradient descent training of GANs as defined in (GOODFELLOW *et al.*, 2014). The number of steps to apply to the discriminator is a hyperparameter k.

for number of training steps do

for k steps do

Sample minibatch of m noise samples  $[\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)}]$  from noise prior  $p_G(\mathbf{z})$ ;

Sample minibatch of m examples  $[\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}]$  from data distribution  $p_{data}(\mathbf{x})$ ;

Update the discriminator by ascending its stochastic gradient:

$$\nabla_{w_D} \frac{1}{m} \sum_{i=1}^{m} \left[ \log D\left(\mathbf{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\mathbf{z}^{(i)}\right)\right)\right) \right];$$

end

Sample minibatch of m noise samples  $[\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)}]$  from noise prior  $p_G(\mathbf{z})$ ; Update the generator by descending its stochastic gradient:

$$\nabla_{w_G} \frac{1}{m} \sum_{i=1}^m \log \left( 1 - D\left( G\left(\mathbf{z}^{(i)}\right) \right) \right);$$

end

In practice, equation 2.3 might not provide sufficient gradient for training G because of the  $\log (1 - D(G(\mathbf{z})))$  term might saturate in the start of training, since D can easily differentiate between the generated data and the actual data. Instead of minimizing this term we may maximize  $\log D(G(\mathbf{z}))$  to give enough gradient for G (GOODFELLOW *et al.*, 2014).

## 3 Instance Space Analysis

In this chapter we will be introducing the novel methodology for algorithm selection and performance evaluation called Instance Space Analysis (ISA), introduced in (MUÑOZ et al., 2018). We will be showing the original definition of an instance space and the adaptation of the methodology brought up by (PAIVA et al., 2022) relating instance hardness.

### 3.1 Instance spaces

ISA is, at its core, an extension of the Algorithm Selection Problem (ASP) (RICE, 1976). Figure 3.1 shows the ISA framework with the ASP highlighted in blue. The objective in the ASP is to automate the process of selecting algorithms based on past similar solved problems. The following sets compose the core of the ASP:

- **Problem Space**  $\mathcal{P}$ : contains all instances of the problem being analysed;
- Instance Sub-space  $\mathcal{I}$ : contains a subset of instances from  $\mathcal{P}$  for which the characteristics and solutions are available;
- Feature Space  $\mathcal{F}$ : a set of descriptive characteristics of the instances in  $\mathcal{I}$ . These are also known as meta-features;
- Algorithm Space A: contains algorithms that may be used to solve the instances in  $\mathcal{I}$ ;
- Performance Space  $\mathcal{Y}$ : contains the performance evaluations of the algorithms in  $\mathcal{A}$  over the instances in  $\mathcal{I}$ ;

The combination of tuples  $(x, f(x), \alpha, y(\alpha, x))$ , where  $x \in \mathcal{I}$ ,  $f(x) \in \mathcal{F}$ ,  $\alpha \in \mathcal{A}$  and  $y(\alpha, x) \in \mathcal{Y}$ , composes a meta-dataset  $\mathcal{M}$ . A meta-learner S can then be trained to select the best algorithm for an instance x based on its meta-features, that is, an algorithm  $\alpha^*$  with maximum predictive performance for x as given by y:

$$\alpha^* = S(f(x)) = \arg\max_{\alpha} ||y(\alpha, x)||. \tag{3.1}$$

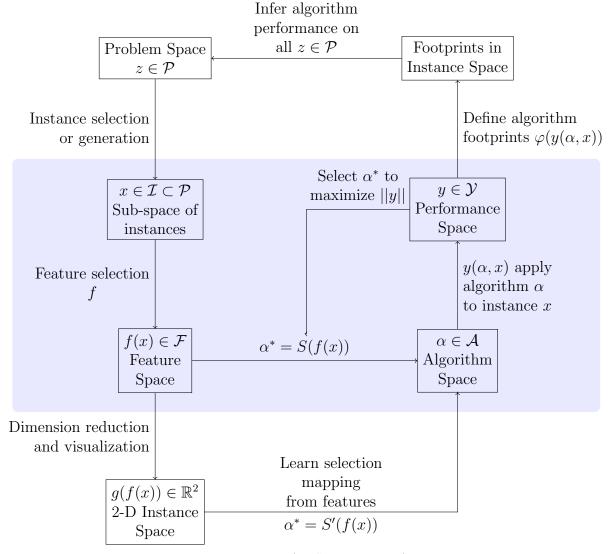


FIGURE 3.1 – ISA framework. Extracted from (MUÑOZ et al., 2018). The ASP is highlighted in blue.

The ISA framework goes further to give insights into why some instances are harder to solve than others, using both the information of meta-features and algorithmic performance in a 2-D embedding, called Instance Space (IS), that can be visually inspected. An optimization problem is solved to find the mapping from meta-features to the IS g(f(x)), such that the distribution of algorithmic performance metrics and meta-features values display as close a linear trend as possible in the IS embedding. This embedding can then be inspected for regions of good and bad algorithmic performance and a new learner can be created to select new algorithms, as in:

$$\alpha^* = S'(g(f(x))) \tag{3.2}$$

In the IS, it is also possible to define algorithm footprints  $\varphi(y(\alpha, x))$ , which are areas where an algorithm  $\alpha$  is expected to perform well. A set of objective measures can be derived from these footprints and aid in the inference of algorithmic performance for other

instances that were not in  $\mathcal{I}$ , such as:

- the area of the footprint A, which can be normalized across multiple algorithms for comparison;
- the density of the footprint  $\rho$ , which can be calculated as the ratio between the number of instances enclosed by the footprint and its area;
- the purity of the footprint p, which is the percentage of instances in the footprint that have good performance.

Summarizing, the application of ISA requires (MUÑOZ et al., 2018):

- 1. building the meta-dataset  $\mathcal{M}$ ;
- 2. reducing the set of meta-features in  $\mathcal{M}$ , keeping only those able to discriminate algorithmic performance;
- 3. creating the 2-D IS from  $\mathcal{M}$ ;
- 4. building the algorithms' footprints in the IS.

#### 3.1.1 Instance Space construction

The problem of finding the optimal mapping between the instance metadata domain to a 2-D IS has been modelled using the Prediction Based Linear Dimensionality Reduction (PBLDR) method (Muñoz et al., 2018). Given a meta-dataset  $\mathcal{M}$  with m meta-features, n instances and a algorithms, let  $F \in \mathbb{R}^{m \times n}$  be the matrix containing the meta-features values for all instances and  $Y \in \mathbb{R}^{n \text{ timesa}}$  be the matrix containing the performance measure of the algorithms on the same instances. The optimal projection is achieved by minimizing the MSE:

$$MSE = ||\mathbf{F} - \hat{\mathbf{F}}||_F^2 + ||\mathbf{Y} - \hat{\mathbf{Y}}||_F^2, \tag{3.3}$$

such that:

$$\mathbf{Z} = \mathbf{A}_r \mathbf{F},\tag{3.4}$$

$$\hat{\mathbf{F}} = \mathbf{B}_r \mathbf{Z},\tag{3.5}$$

$$\hat{\mathbf{Y}}^T = \mathbf{C}_r \mathbf{Z}.\tag{3.6}$$

Where  $\mathbf{A}_r \in \mathbb{R}^{2 \times m}$ ,  $\mathbf{B}_r \in \mathbb{R}^{m \times 2}$  and  $\mathbf{C}_r \in \mathbb{R}^{a \times 2}$ .  $\mathbf{Z} \in \mathbb{R}^{2 \times n}$  is the matrix of instance coordinates in the IS and  $A_r$  is the projection matrix. (PAIVA *et al.*, 2022) solves this problem numerically using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm.

#### 3.1.2 Footprint analysis

As said before, a footprint is a region in the IS where an algorithm is expected to perform well based on inference from empirical performance analysis (MUÑOZ et al., 2018). (PAIVA et al., 2022) goes into more detail of its construction, qualitatively we can infer from the set of footprint measures defined before that a good algorithm will have large quantities of each of those measures, i.e. a large area shows that an algorithm performs well in a large portion of the IS, a large density shows that the footprint contains a large amount of instances and a large purity shows that the algorithm performs well in most instances.

## 3.2 ISA for a single dataset

In (Muñoz et al., 2018), ISA is defined with an instance being an entire classification dataset. (PAIVA et al., 2022) has adapted the framework and reduced the problem space  $\mathcal{P}$  into a single dataset, with each instance being an observation inside the dataset. This has come with the removal of some steps of the original ISA, namely the algorithmic recommendation module and the creation of new instances from the IS.

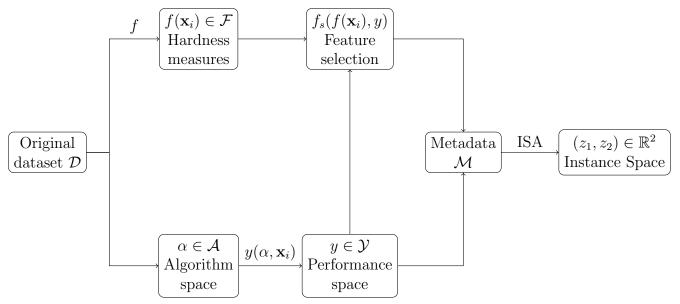


FIGURE 3.2 - ISA framework for a single dataset. Extracted from (PAIVA et al., 2022).

Given a classification dataset  $\mathcal{D}$  with  $n_D$  instances  $\mathbf{x}_i$ ,  $m_D$  input features and each

instance labelled in a class  $y_i$ , we have:

- Problem space  $\mathcal{P}$ : reduced to the dataset  $\mathcal{D}$ ;
- Instance sub-space  $\mathcal{I}$ : contains all individual instances  $\mathbf{x}_i$ ;
- Feature space  $\mathcal{F}$ : contains a set of meta-features known as hardness measures.

The modified framework is shown in figure 3.2. For each instance, a set of hardness measures are stored in  $\mathcal{F}$ , and each algorithm  $\alpha \in \mathcal{A}$  is evaluated over the instance  $\mathbf{x}_i$  and has its performance  $y(\alpha, \mathbf{x}_i)$  measured and stored in  $\mathcal{Y}$ . The measure used is a cross-validated log-loss error obtained in the prediction of the instance label. A feature selection is used with these measures and the hardness measures, resulting in a reduced feature set  $f_s(f(\mathbf{x}_i), y)$ .

Combining the reduced feature set to the predictive performance of the algorithms allows us to construct the meta-dataset  $\mathcal{M}$ , from which the IS is extracted. The steps are explained in (PAIVA *et al.*, 2022), we will summarize some important topics.

#### 3.2.1 Hardness measures

(PAIVA et al., 2022) revisits the definition of *Instance Hardness* (IH), a property that indicates the probability of an instance being misclassified given a classification hypothesis:

$$IH_h(\mathbf{x}_i, y_i) = 1 - p(y_i|\mathbf{x}_i, h), \tag{3.7}$$

where  $h: X \to Y$  is a classification hypothesis mapping an input space of features X to an output space of labels Y. In practice, h is a learning algorithm induced from the dataset  $\mathcal{D}$  and hyperparameters  $\beta$ , that is  $h = l(\mathcal{D}, \beta)$ . We can then compute the IH of the whole algorithm space  $\mathcal{A}$ :

$$IH_{\mathcal{A}}(\mathbf{x}_i, y_i) = 1 - \frac{1}{|\mathcal{A}|} \sum_{l \in \mathcal{A}} p(y_i | \mathbf{x}_i, l(\mathcal{D}, \beta)). \tag{3.8}$$

The idea is that instances frequently misclassified over the algorithm space can be considered hard, and instances being correctly classified are considered easy. (PAIVA et al., 2022) also shows a set of hardness metrics being extracted for each instance. Table 3.1 lists the measures used, the formal definition for each one is shown in Appendix A.

Measure	Acronym	Min.	Max.
k-Disagreeing Neighbors	kDN	0	1
Disjunct Class Percentage	DCP	0	1
Tree Depth (pruned)	$TD_P$	0	1
Tree Depth (unpruned)	$TD_U$	0	1
Class Likelihood	CL	0	1
Class Likelihood Difference	CLD	0	1
Fraction of features in overlapping areas	F1	0	1
Fraction of nearby instances different class	N1	0	1
Ratio of intra-extra class distances	N2	0	$\approx 1$
Local set cardinality	LSC	0	1
Local set radius	LSR	0	1
Usefulness	U	$\approx 0$	1
Harmfulness	Н	0	$\approx 1$

TABLE 3.1 – Hardness measures used in (PAIVA et al., 2022).

#### 3.2.2 Performance assessment

To assess the performance from each algorithm in the dataset  $\mathcal{D}$ , it is first split into r folds according to the cross-validation strategy such that each instance from the dataset belongs to only one fold. r-1 folds are used for training the algorithm while the last fold is used for testing. Therefore we can compute a performance estimate for each instance and algorithm combination. Repeating this process yields an interval estimation (PAIVA et al., 2022). The measure used for performance assessment was the log-loss, or cross-entropy, defined in equation 3.9:

$$\log \log(\mathbf{x}_i) = -\sum_{c=1}^{C} y_{i,c} \log(p_{i,c}), \tag{3.9}$$

where C is the number of classes the problem has,  $y_{i,c}$  is a binary indicator of whether the class c is an actual label of  $\mathbf{x}_i$  or not and  $p_{i,c}$  is the probability that the classifier attributes  $\mathbf{x}_i$  to class c.

#### 3.2.3 Feature selection

For feature selection, (PAIVA et al., 2022) employs a method called Minimum Redundancy Maximum Relevance (MRMR), a criterion that gradually reduces the effect of feature redundancy as more features are selected. There is a trade-off between minimizing the number of redundant features and keeping relevant features, this method rejects redundant features at first but tolerates redundancy as more informative features are added. The mathematical model for MRMR is in equation 3.10:

$$J(\mathbf{f}_k) = MI(\mathbf{f}_k; \mathbf{y}_j) - \frac{1}{|\mathcal{S}_j|} \sum_{\mathbf{f}_i \in \mathcal{S}_j} MI(\mathbf{f}_k; \mathbf{f}_i),$$
(3.10)

where  $J(\mathbf{f}_k)$  is a score for the k-th feature vector  $\mathbf{f}_k$ ,  $MI(\mathbf{f}_k; \mathbf{y}_j)$  is the mutual information between the feature vector and the response variable for the j-th algorithm and  $S_j$  is the set of selected features for the j-th algorithm.  $S_j$  is initially empty and the first feature chosen is the one with maximum mutual information between the feature vector and the response variable  $\mathbf{y}_j$ . Features are selected based on their score in subsequent rounds until there are a desired number of features chosen  $n_f = |S_j|$ 

#### 3.2.4 IS representation and footprints

Given the now constructed meta-dataset  $\mathcal{M}$  after feature selection and performance assessments, the 2-D IS can be constructed. (PAIVA *et al.*, 2022) added a rotation to the IS so that bad instances are placed towards the upper left of the IS, while good instances are placed towards the bottom right.

All of this section is implemented in the Python library PyHard (PAIVA et al., 2022). This work will use this implementation for reproducing this methodology.

## 4 Methodology

In this chapter, we will describe the problem's modelling and the main tools being used.

## 4.1 Instance Space generation

For the IS generation, we will use the PyHard (PAIVA et al., 2022) library. The library has some examples of the implementation, those being discussed in the paper (PAIVA et al., 2022). In this work we will generate the IS, attach the resulting 2-D embedding with the original dataset  $\mathcal{D}$  and feed into the GAN architecture as training data.

#### 4.2 Generator and Discriminator creation

The implementation of the GAN model is straightforward. Using the PyTorch (PASZKE et al., 2019) framework we can define classes that function as neural network models. It has methods for backpropagation and has multiple optimizers implemented. We will be using the Adam optimizer (KINGMA; BA, 2017). The training algorithm in algorithm 1 will be used, with the optimization step of G being the maximization of  $\log D(G(\mathbf{z}))$  for better gradients.

The optimization step for D will be done in two parts. Firstly, we will use real samples from the training set, forward pass through D, calculate the loss  $(\log(D(x)))$ , then calculate the gradients with backpropagation. Secondly, we will use the fake samples from the current generator, forward pass them through D, calculate the loss  $(\log(1-D(G(z))))$ , and accumulate the gradients with backpropagation.

## 4.3 Re-evaluation of the generated data

After training the generator G, we will re-evaluate the generated data using the adapted ISA. We will use the generated 2-D embedding and check if it correlates with the

 $2\text{-}\mathrm{D}$  embedding computed from the generated data.

# 5 Results

## 5.1 Planned results

# 6 Conclusion

- 6.1 Preliminary conclusions and future work
- 6.2 Work plan

# **Bibliography**

- GOODFELLOW, I.; POUGET-ABADIE, J.; MIRZA, M.; XU, B.; WARDE-FARLEY, D.; OZAIR, S.; COURVILLE, A.; BENGIO, Y. Generative adversarial nets. *In*: GHAHRAMANI, Z.; WELLING, M.; CORTES, C.; LAWRENCE, N.; WEINBERGER, K. (Ed.). **Advances in Neural Information Processing Systems. Proceedings** [...]. Curran Associates, Inc., 2014. v. 27. Available at: https://proceedings.neurips.cc-/paper\_files/paper/2014/file/5ca3e9b122f61f8f06494c97b1afccf3-Paper.pdf.
- HORNIK, K.; STINCHCOMBE, M.; WHITE, H. Multilayer feedforward networks are universal approximators. **Neural Networks**, v. 2, n. 5, p. 359–366, 1989. ISSN 0893-6080. Available at: https://www.sciencedirect.com/science/article/pii/0893608089900208.
- KINGMA, D. P.; BA, J. Adam: A Method for Stochastic Optimization. 2017. Available at: https://doi.org/10.48550/arXiv.1412.6980.
- MUNOZ, M. A.; VILLANOVA, L.; BAATAR, D.; SMITH-MILES, K. Instance spaces for machine learning classification. **Machine Learning**, v. 107, n. 1, p. 109–147, Jan 2018. ISSN 1573-0565. Available at: https://doi.org/10.1007/s10994-017-5629-5.
- PAIVA, P. Y. A.; MORENO, C. C.; SMITH-MILES, K.; VALERIANO, M. G.; LORENA, A. C. Relating instance hardness to classification performance in a dataset: a visual approach. **Machine Learning**, v. 111, n. 8, p. 3085–3123, Aug 2022. ISSN 1573-0565. Available at: https://doi.org/10.1007/s10994-022-06205-9.
- PASZKE, A.; GROSS, S.; MASSA, F.; LERER, A.; BRADBURY, J.; CHANAN, G.; KILLEEN, T.; LIN, Z.; GIMELSHEIN, N.; ANTIGA, L.; DESMAISON, A.; KÖPF, A.; YANG, E.; DEVITO, Z.; RAISON, M.; TEJANI, A.; CHILAMKURTHY, S.; STEINER, B.; FANG, L.; BAI, J.; CHINTALA, S. **PyTorch: An Imperative Style, High-Performance Deep Learning Library**. 2019. Available at: https://doi.org/10.48550/arXiv.1912.01703.
- PURI, M.; SOLANKI, A.; PADAWER, T.; TIPPARAJU, S. M.; MORENO, W. A.; PATHAK, Y. Introduction to artificial neural network (ann) as a predictive tool for drug design, discovery, delivery, and disposition: Basic concepts and modeling. **Artificial Neural Network for Drug Design, Delivery and Disposition**, Elsevier Inc., p. 3–13, 2016.
- RICE, J. R. The algorithm selection problem. *In*: RUBINOFF, M.; YOVITS, M. C. (Ed.). Elsevier, 1976, (Advances in Computers, v. 15). p. 65–118. Available at: https://www.sciencedirect.com/science/article/pii/S0065245808605203.

# Appendix A - Instance Hardness

A.1 Metrics used in subsection 3.2.1

	FOLHA DE REGIST	TRO DO DOCUMENTO	
1. CLASSIFICAÇÃO/TIPO TC	<ul> <li>DATA</li> <li>23 de junho de 2023</li> </ul>	3. DOCUMENTO Nº DCTA/ITA/DM-018/2015	<sup>4.</sup> № DE PÁGINAS 31
<sup>5.</sup> TÍTULO E SUBTÍTULO: Use of generative neural ne	tworks for instance space coo	diffication and generation of da	ta with specific properties
6. AUTOR(ES):  Gabriel Barbosa Martinz			
7. INSTITUIÇÃO(ÕES)/ÓRGÂ Instituto Tecnológico de Ae	ÃO(S) INTERNO(S)/DIVISÃO(Ĉ eronáutica – ITA	ĎES):	
8. PALAVRAS-CHAVE SUGER Cupim; Cimento; Estrutura			
9. PALAVRAS-CHAVE RESUL Cupim; Dilema; Construção	*		
<sup>10.</sup> APRESENTAÇÃO:		$(\mathbf{X})$	Nacional () Internacional
Trabalho de Graduação, IT	'A, São José dos Campos, 20	15. 31 páginas.	
juntas ou graus de liberda ou como resultado de pro- pelo movimento das junt A utilização de redundâr consumo de energia, por e do totalmente atuado, em apresentamos a modelager índice é utilizado na sequé seja maior que o número	ade do sistema são equipado jeto. As juntas passivas de as ativas usando as caracteria de atuação das juntas exemplo. Apesar da estrutur geral suas caraterísticas dinâm dinâmica de um manipuladência de controle ótimo do m de passivas $(n_a > n_p)$ perma má mais entradas (torques no	D termo subatuado se refere a se com atuadores, o que ocorre manipuladores desse tipo são erísticas de acoplamento da de ativas permite a minimização ca cinemática de manipuladore micas diferem devido a presenção subatuado e o conceito de franipulador. A hipótese de que ite o controle ótimo das juntas atuadores das juntas ativas)	e na prática devido a falhas o indiretamente controladas inâmica de manipuladores. o de alguns critérios, como es subatuados ser idêntica a a de juntas passivas. Assim, indice de acoplamento. Este e o número de juntas ativas s passivas, uma vez que na
12. GRAU DE SIGILO: (X) OSTENS	IVO () RESE	RVADO () SEC	CRETO