## 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** 

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

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# 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 Uno	lergrad	luation	$\operatorname{Study}$
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## **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 a neuron	17
FIGURE 2.2 –	A model of a simple fully-connected neural network with 3 inputs, 3 outputs and a hidden layer with 4 nodes	18
FIGURE 2.3 –	Flowchart of the GAN training model	19
FIGURE 3.1 –	ISA framework. Extracted from (MUÑOZ et al., 2018). The ASP is highlighted in blue	22
FIGURE 3.2 –	ISA framework for a single dataset. Extracted from (PAIVA et al., 2022)	24
FIGURE A.1 -	-Uma figura que está no apêndice	30

# List of Tables

## List of Abbreviations and Acronyms

CTq computed torque

DC direct current

EAR Equação Algébrica de Riccati

GDL graus de liberdade

ISR interrupção de serviço e rotina LMI linear matrices inequalities

MIMO multiple input multiple output

PD proporcional derivativo

PID proporcional integrativo derivativo

PTP point to point

UARMII Underactuated Robot Manipulator II

VSC variable structure control

# List of Symbols

# **Contents**

1	Int	RODUCTION	14
	1.1	Motivation	. 14
	1.2	Objective	. 15
	1.3	Scope	. 15
	1.4	Outline of this work	. 15
2	Ma	CHINE LEARNING	16
	2.1	Classification	. 16
	2.2	Neural networks	. 16
	2.2	.1 Artificial neuron	. 17
	2.2	.2 The network	. 17
	2.2	.3 Learning	. 18
	2.3	Generative Adversarial Networks	. 19
3	Ins	TANCE SPACE ANALYSIS	21
	3.1	Instance spaces	. 21
	3.1	.1 Instance Space construction	. 23
	3.1	.2 Footprint analysis	. 24
	3.2	ISA for a single dataset	. 24
4	ME	THODOLOGY	25
5	Res	SULTS	26
	<b>5.1</b>	Planned results	. 26

CONTENTS	xiii
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6.1	Preliminary conclusions and future work	27
6.2	Work plan	27
Biblio	GRAPHY	28
APPEN	DIX A – TÓPICOS DE DILEMA LINEAR	30
<b>A.</b> 1	Uma Primeira Seção para o Apêndice	30
Annex	A - Exemplo de um Primeiro Anexo	31
A.1	Uma Secão do Primeiro Anexo	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).

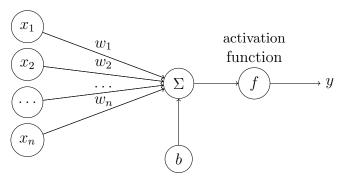


FIGURE 2.1 – Model of a neuron.

#### 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.

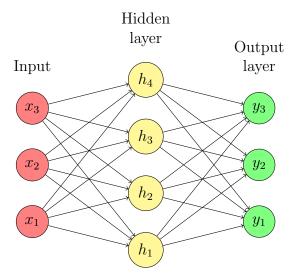


FIGURE 2.2 – A model of a simple fully-connected neural network with 3 inputs, 3 outputs and a hidden layer with 4 nodes.

#### 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).

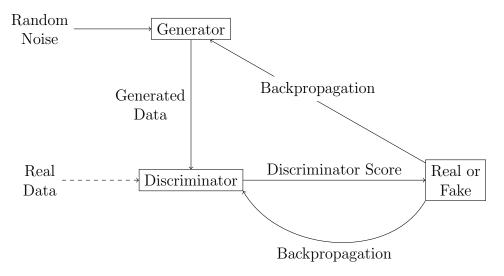


FIGURE 2.3 – Flowchart of the GAN training model.

**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:

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

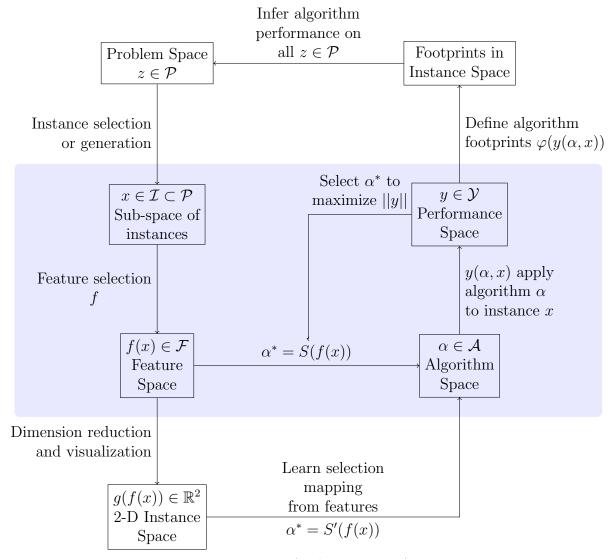


FIGURE 3.1 – ISA framework. Extracted from (MUÑOZ et al., 2018). The ASP is highlighted in blue.

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:

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

such that:

$$Z = A_r F, (3.4)$$

$$\hat{F} = B_r Z,\tag{3.5}$$

$$\hat{Y}^T = C_r Z. (3.6)$$

Where  $A_r \in \mathbb{R}^{2 \times m}$ ,  $B_r \in \mathbb{R}^{m \times 2}$  and  $C_r \in \mathbb{R}^{a \times 2}$ .  $Z \in \not\models \times \times$  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.

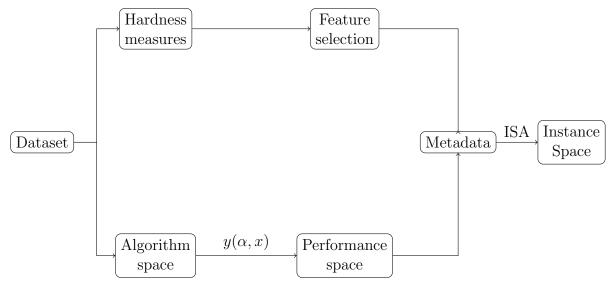


FIGURE 3.2 – ISA framework for a single dataset. Extracted from (PAIVA et al., 2022).

# 4 Methodology

# 5 Results

## 5.1 Planned results

# 6 Conclusion

- 6.1 Preliminary conclusions and future work
- 6.2 Work plan

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## Appendix A - Tópicos de Dilema Linear

## A.1 Uma Primeira Seção para o Apêndice

A matriz de Dilema Linear M e o vetor de torques inerciais b, utilizados na simulação são calculados segundo a formulação abaixo:

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix}$$
 (A.1)



FIGURE A.1 – Uma figura que está no apêndice

# Annex A - Exemplo de um Primeiro Anexo

## A.1 Uma Seção do Primeiro Anexo

Algum texto na primeira seção do primeiro anexo.

	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
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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