## A (very short) introductory journey through data science

2022 International Workshop in Applied Statistics and Data Science (Cartagena – Colombia)

June 29 – July 1, 2022

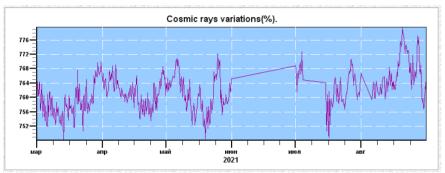


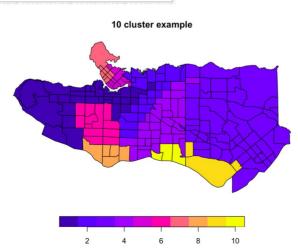
#### **Contents**

We are talking about three important topics (or common task) in Data Sciene:

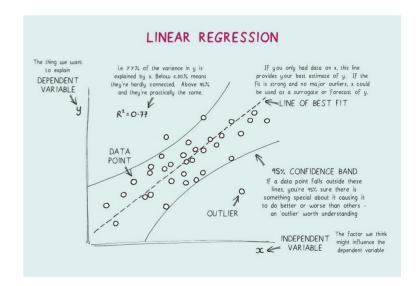
## Imputation methods

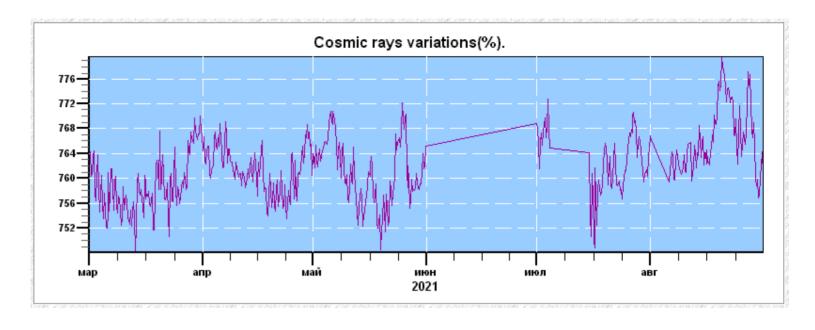
**Clustering methods** 





## **Regression methods**





## **Tutorial: Introduction to Missing Data Imputation**





# $131 \rightarrow 12$ $241 \rightarrow 24$ $162 \rightarrow 36$ $343 \rightarrow 48$ $146 \rightarrow ??$



## $111 \rightarrow 12$ $231 \rightarrow 24$ $324 \rightarrow 36$ $453 \rightarrow 48$ $542 \rightarrow ??$

# Think fast 1...

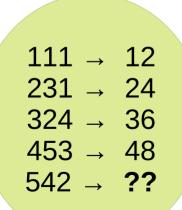
131	$\rightarrow$	12
241	$\rightarrow$	24
162	$\rightarrow$	36
343	$\rightarrow$	48
146	$\rightarrow$	??

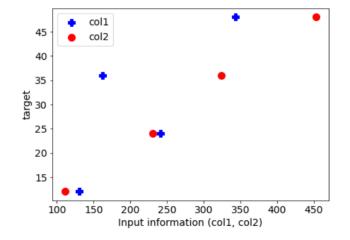
	col1	col2	targ
0	131	111	12
1	241	231	24
2	162	324	36
3	343	453	48
4	146	542	??

0LS	Regression	Results

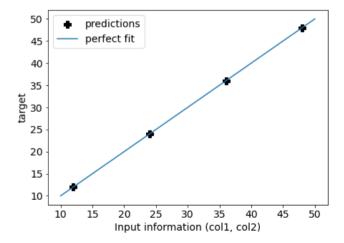
	======		====				
Dep. Variable:		ta	rg	R-square	ed:		1.000
Model:		0	LS	Adj. R-9	squared:		1.000
Method:	L	east Squar	es	F-statis	stic:		1.319e+05
Date:	Mon,	27 Jun 20	22	Prob (F-	-statistic):		0.00195
Time:		08:56:	49	Log-Like	elihood:		8.9039
No. Observations:			4	AIC:			-11.81
Df Residuals:			1	BIC:			-13.65
Df Model:			2				
Covariance Type:		nonrobu	st				
	coef	std err		t	P> t	[0.025	0.975]
const 1.	2792	0.075	17	. 113	0.037	0.329	2.229
col1 -0.	0160	0.001	-30	. 284	0.021	-0.023	-0.009
col2 0.	1152	0.000	333	.744	0.002	0.111	0.120







Model: targ ~ col1 + col2,



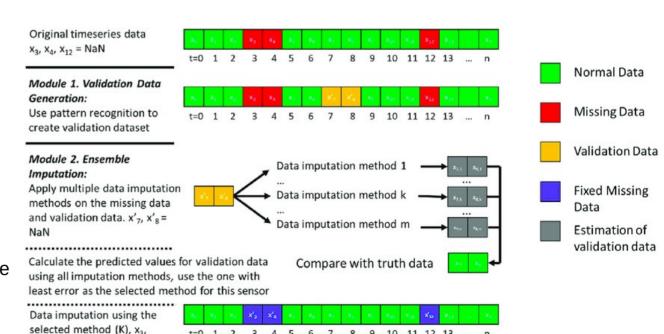
target(predcition) = 61

## Missing data mechanisms

The study of missing data was formalized by Donald Rubin (see [6], [5]) with the concept of missing mechanism in which missing-data indicators are random variables and assigned a distribution. Missing data mechanism describes the underlying mechanism that generates missing data and can be categorized into three types — missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR). Informally speaking, MCAR means that the occurrence of missing values is completely at random, not related to any variable. MAR implies that the missingness only relate to the observed data and NMAR refers to the case that the missing values are related to both observed and unobserved variable and the missing mechanism cannot be ignored.

 $x_4, x_{12} \neq NaN$ 

Missing data is a common problem in practical data analysis. They are simply observations that we intend to make but did not. In datasets, missing values could be represented as '?', 'nan', 'N/A', blank cell, or sometimes '-999', 'inf', '-inf'. The aim of this tutorial is to provide an introduction of missing data and describe some basic methods on how to handle them.



April 30, 2021

Dataset Open Access

## Water-quality data imputation with a high percentage of missing values: a machine learning approach

Rafael Rodríguez; Marcos Pastorini; Lorena Etcheverry; Christian Chreties; Mónica Fossati; Alberto Castro;
Angela Gorgoglioge

The monitoring of surface-water quality followed by water-quality modeling and analysis is essential for generating effective strategies in water resource management. However, water-quality studies are limited by the lack of complete and reliable data sets on surface-water-quality variables. These deficiencies are particularly noticeable in developing countries.

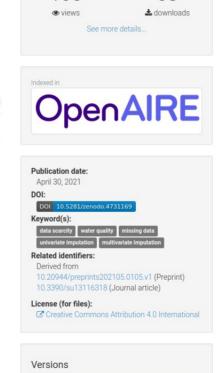
This work focuses on surface-water-quality data from Santa Lucía Chico river (Uruguay), a mixed lotic and lentic river system. Data collected at six monitoring stations are publicly available at https://www.dinama.gub.uy/oan/datos-abiertos/calidad-agua/. The high temporal and spatial variability that characterizes water-quality variables and the high rate of missing values (between 50% and 70%) raises significant challenges.

To deal with missing values, we applied several statistical and machine-learning imputation methods. The competing algorithms implemented belonged to both univariate and multivariate imputation methods (inverse distance weighting (IDW), Random Forest Regressor (RFR), Ridge (R), Bayesian Ridge (BR), AdaBoost (AB), Huber Regressor (HR), Support Vector Regressor (SVR), and K-nearest neighbors Regressor (KNNR)).

IDW outperformed the others, achieving a very good performance (NSE greater than 0.8) in most cases.

In this dataset, we include the original and imputed values for the following variables:

- Water temperature (Tw)
- · Dissolved oxygen (DO)
- Electrical conductivity (EC)
- pH
- Turbidity (Turb)
- Nitrite (NO2-)
- Nitrate (NO3-)
- Total Nitrogen (TN)



38

105

#### https://www.mdpi.com/2071-1050/13/11/6318

Open Access Article

## Water-Quality Data Imputation with a High Percentage of Missing Values: A Machine Learning Approach

by & Rafael Rodriguez 1 © 0, & Marcos Pastorini 2 © 0, & Lorena Etcheverry 2 © 0, & Christian Chreties 1 ©, & Monica Fossati 1 ©, & Alberto Castro 2 © 0 and Angela Gorgogilone 1.\* © 0

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Academic Editor: Ashwani Kumar Tiwari

Sustainability 2021, 13(11), 6318; https://doi.org/10.3390/su13116318

Received: 3 May 2021 / Revised: 30 May 2021 / Accepted: 1 June 2021 / Published: 2 June 2021

(This article belongs to the Special Issue Water Quality: Current State and Future Trends)

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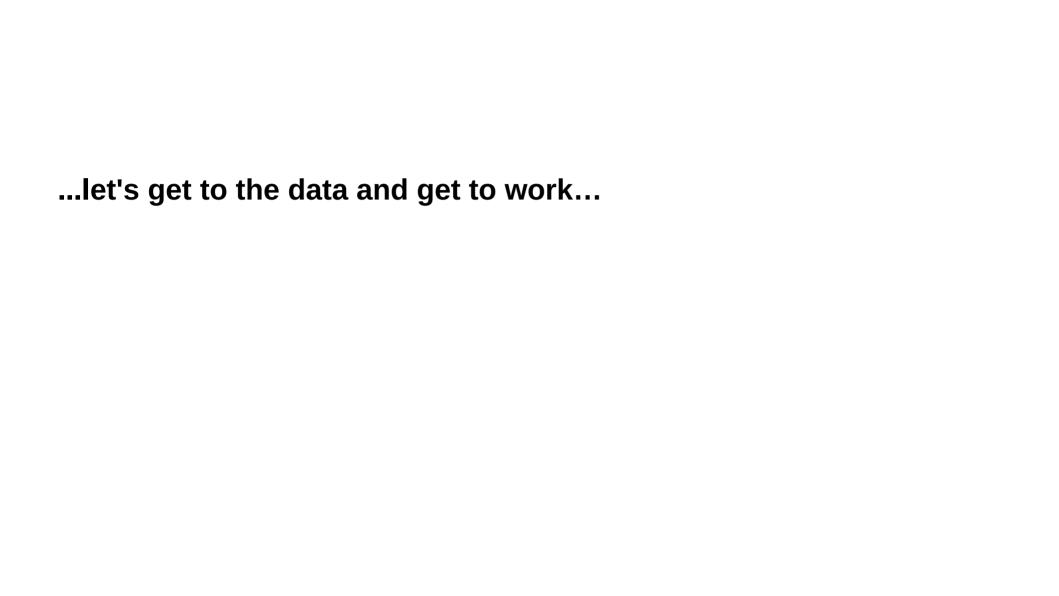
#### Abstract

The monitoring of surface-water quality followed by water-quality modeling and analysis are essential for generating effective strategies in surface-water-resource management. However, worldwide, particularly in developing countries, water-quality studies are limited due to the lack of a complete and reliable dataset of surface-water-quality variables. In this context, several statistical and machine-learning models were assessed for imputing water-quality data at six monitoring stations located in the Santa Lucia Chico river (Uruguay), a mixed lotic and lentic river system. The challenge of this study is represented by the high percentage of missing data (between 50% and 70%) and the high temporal and spatial variability that characterizes the water-quality variables. The competing algorithms implement univariate and multivariate imputation methods (inverse distance weighting (IDW), Random Forest Regressor (RFR), Ridge (R), Bayesian Ridge (R), AdaBoost (AB), Hubber Regressor (HR), Support Vector Regressor (SVR) and K-nearest neighbors Regressor (KNNTS). According to the results, more than 75% of the imputation outcomes are considered "satisfactory" (NSE > 0.45). The imputation performance shows better results at the monitoring stations located inside the reservoir than those positioned along the mainstream. IDW was the model with the best imputation results, followed by RFR, HR and SVR. The approach proposed in this study is expected to aid water-resource researchers and managers in augmenting water-quality datasets and overcoming the missing data issue to increase the number of future studies related to the water-quality mater-quality datasets and overcoming the missing data issue to increase the number of future studies related to the water-quality mater-quality datasets and overcoming the missing data issue to increase the number of future studies related to the water-quality

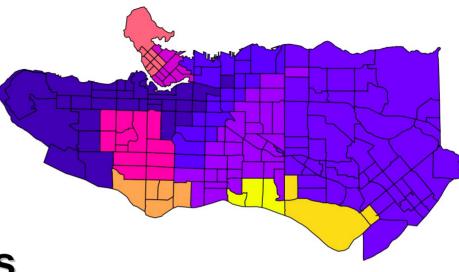
Keywords: data scarcity; water quality; missing data; univariate imputation; multivariate imputation; machine learning hydroinformatics

▼ Show Figures

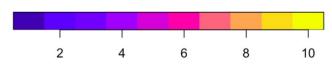
https://zenodo.org/record/4731169#.YrmoADXMJ8s



#### 10 cluster example



**Clustering methods** 





## **Regression methods**

