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ASTUTENESS PROJECT

AI-Driven Tools in Healthcare: A Visual Trustworthy Treatment Decision Support Systems

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SD for Machine Learning Explainability: Progress Report

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Contents

Background

ANTIMICROBIAL RESISTANCE PROBLEM (ARP)
AR: the ability of microorganisms to become resistant to antibiotics.

EUROPE: ARP causes of 33,000 deaths/year and to be 1,500 M€ (ECDC)
Spain 2,500 deaths per annum, and an additional health expenditure of 150M€ /year [Spanish Agencey of Drugs report 2020]

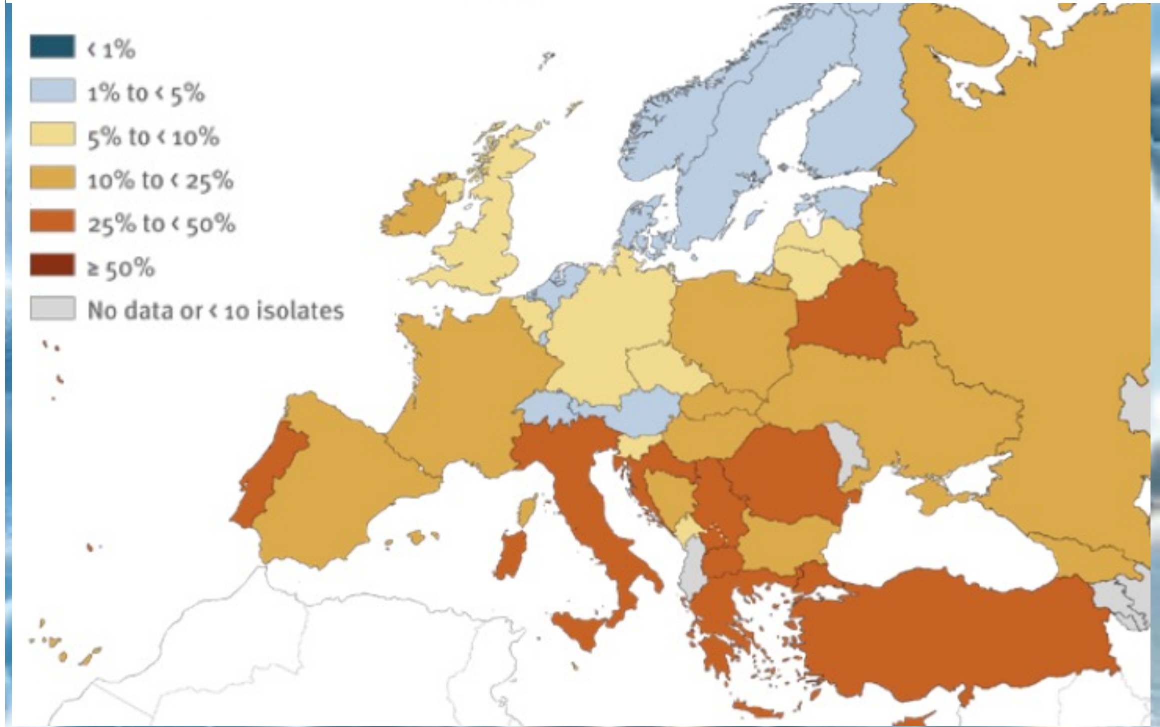
1 of the 6 priority strategic lines of the Spanish Plan against Antibiotic Resistance (PRAN): **surveillance of resistant bacteria** and the consumption of antibiotics in hospitals.

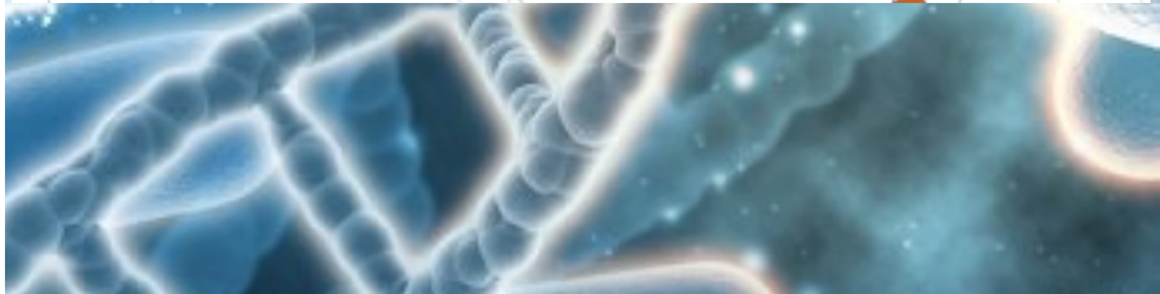
One of the main scenarios of this strategic line is the improvement to the **prescription of antibiotics.**

For this, we intend to predict the Minimum Inhibitory Concentration (**MIC**) of the bacteria to a given treatment using the data from their hospital stay.

Antimicrobial resistance surveillance in Europe 2022 by ECDC + WHO

S. aureus: percentage of invasive isolates resistant to methicillin (MRSA)





Picture (CC0) https://www.freepik.es/foto-gratis/adn-bacterias_923816.htm#query=BACTERIA&position=2&from_view=search&track=sph&uuid=cea4540f-c9b0-4bfe-974b-4839b2d99054

Dataset Open-Data MIMIC-III

MIMIC-III[1] ('Medical Information Mart for Intensive Care') is a large, single-center database of patients admitted to ICU at a large tertiary care hospital.

We use a smaller data **subset** containing information for cultures treated with **Vancomycin**.

Variables: patient gender and age, previous Vancomycin treatments, admission type and location, **culture_susceptibility,** etc.

[1] Johnson, A., Pollard, T., Shen, L. *et al.* MIMIC-III, a freely accessible critical care database. *Sci Data* **3**, 160035 (2016). https://doi.org/10.1038/sdata.2016.35

Our data

Our data consists of 531 instances of 26 variables.

We aim to predict the **culture susceptibility** (**R**esistant/**S**usceptible)

We observe that our data is highly unbalanced

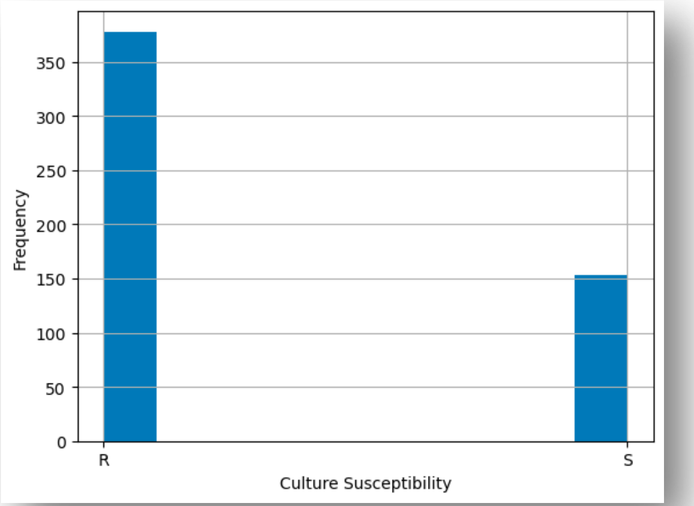
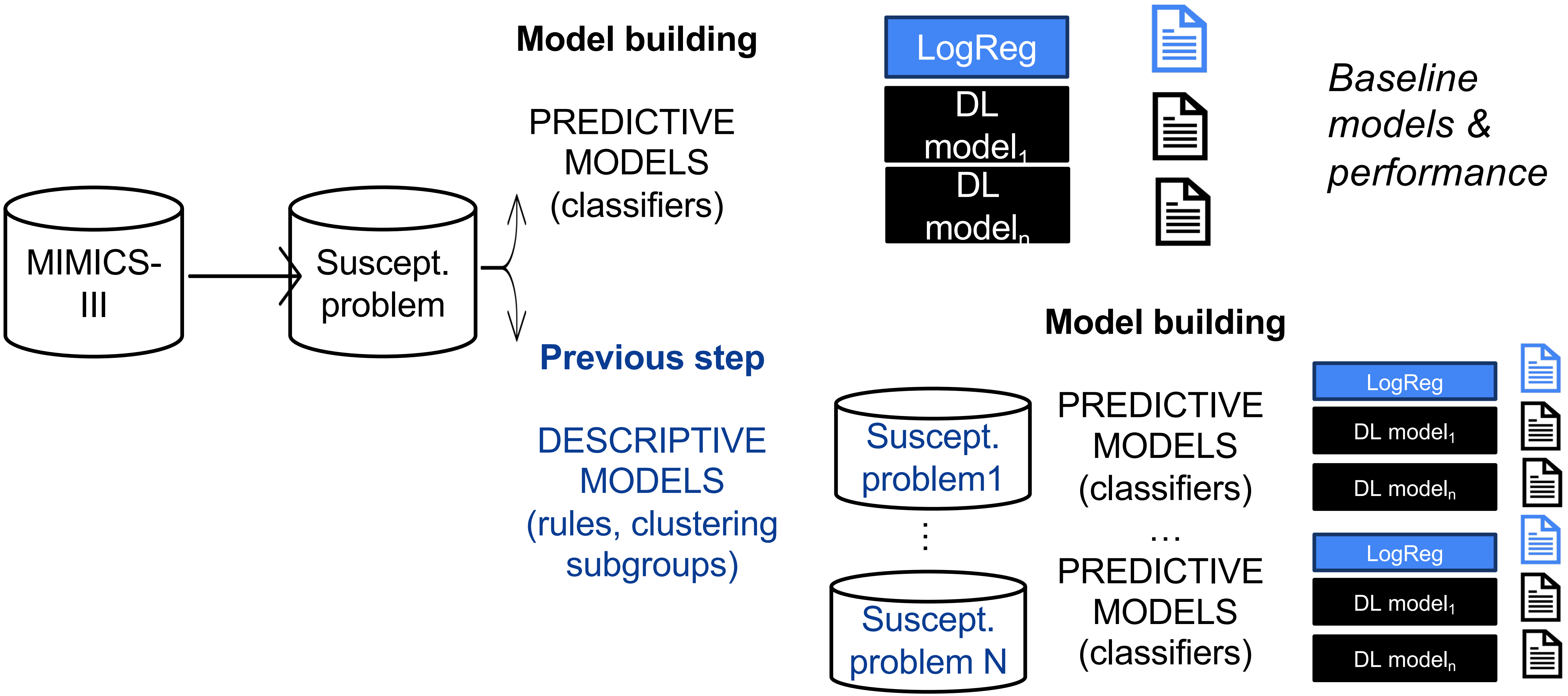
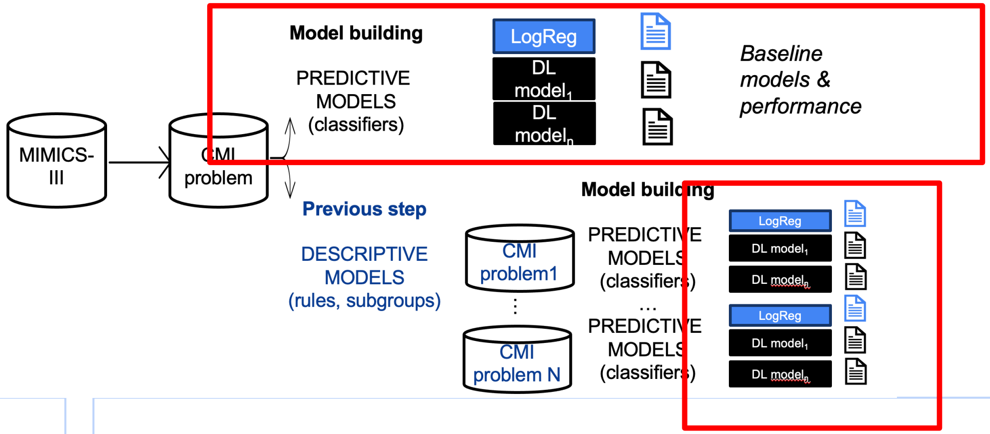


Figure 1: Culture susceptibility histogram

Methodology



Methodology. Predictive models



MODELS ANALYSIS

TESTING ML MODELS CAPACITY TO PRODUCE PREDICTORS

LOGIT

regularization applied

Tree-based & ensembles

RANDOM FOREST

deep trees (overfit individually)
- quality of split: gini
- samples to split node: 2
- depth: until leaves are pure
- samples to be leaf: 1

bootstrap to build trees

no class/individual weights

GRADIENT BOOSTING TREES

number estimators (stages) = 100

trees:
- samples to split node: 2 (quality split MSE)
- depth: max. 3 (weak classifiers)
- samples to be leaf: 1
- # leaf nodes: no limits

no class/individual weights

Kernel and NN-based

SVM CLASSIFIER

multi-class classification= 1vs1 scheme

kernel:
- rbf kernel
- max. degree function: 3
- coefficient gamma = 1 / (n_features * X.var())

no class weights

SIMPLE NNs

architecture

-1,2,3 layer

-16, 32, 64 neurons

-sigmoid, tanh, relu activation

-loss: binary cross entropy

grid search of hyperparameters

epochs=10

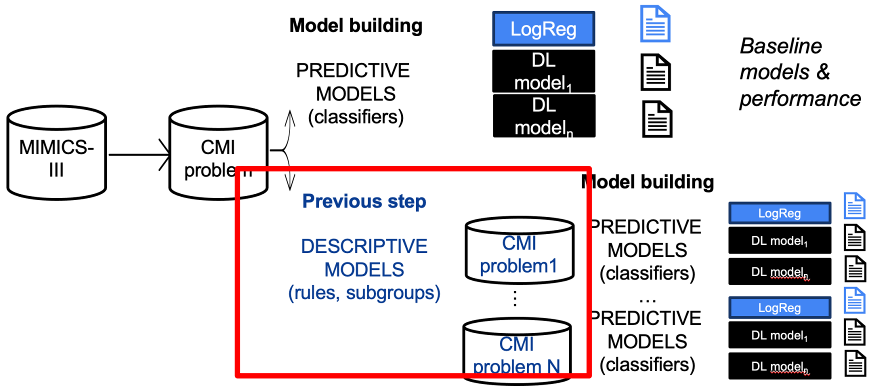
Results. Baseline models

- High accuracy for Resistant events, low accuracy for Susceptible events.
- All the models have similar behaviors.

	accuracy	specificity	sensitivity	f1	balanced_accuracy
LOGIT	0,8644	0,9974	0,5346	0,6853	0,766
R-forest	0,8494	0,9683	**0,5542**	0,6734	0,7612
GB	0,8531	0,9735	0,5538	0,6758	0,7636
SVM	0,8625	**1**	0,5221	0,6784	0,761
NN	**0,8682**	**1**	0,5412	**0,6937**	**0,7706**

Table 2: Baseline models results

Methodology. Descriptive Models



- Algorithm: BSD (define total amount of subgroups)
- Discretization of continuous variables using median as threshold
- Parameters:
  - Number of subgroups: 10
  - Quality measure: WRAcc and Qc
  - Minimum support: ~1/3 of total events in the target
  - Max depth: 6
  - Target: Response = Resistant and Response = Susceptible
- We generate a data subset using each rule (20 new dataset)

Results. Generated datasets

- For each rule, we generate a dataset containing only the instances that follow the rule.
- With this, we obtain 20 data subsets from the original dataset.
- We remove the categorical columns that appear in the rule (since they are now constant).
- The number of rows for each data subset is equal to the subgroup support (tp +fp)

Future work

- Deal with rows in multiple partitions
- Deal with rows not present in any partitions
- Apply conventional pattern mining techniques