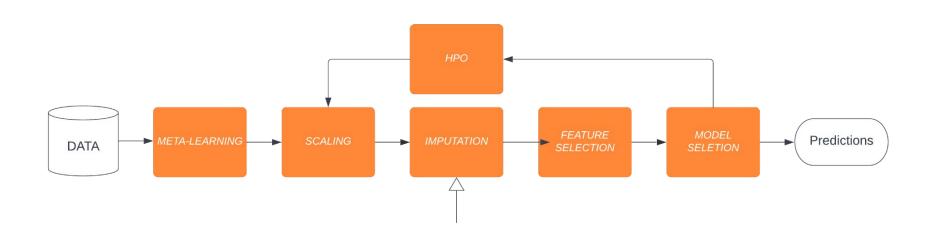
Missing data

Udemy course

Why is it a problem?

- Many machine learning algorithms require complete data sets.
- Different types of missing data may require different methods.
- Mostly studied by statisticians and not by ML scientists.
- Literature reports contradicting results.

Imputation in the AutoML pipeline



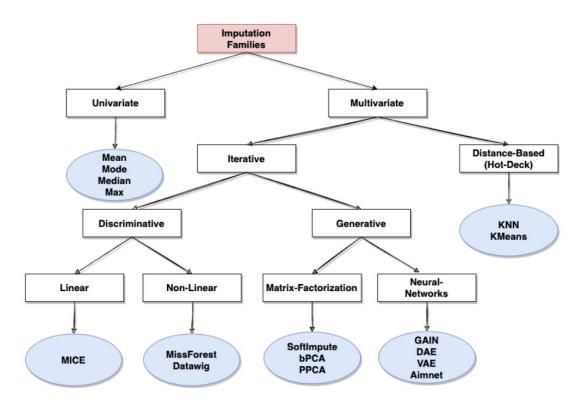
Imputation in AutoML tools

Tool	Simple-Imp.	SoftImpute	MissForest	New cat.	Other
JadBio	✓				
ТРОТ	✓				
AutoPrognosis	~	~	~		~
AutoGluon	✓			~	
AutoSklearn	✓				~

Missingness mechanisms

- Missing Completely at Random (MCAR): Missing values don't depend on the data.
 - E.g : A dataset got corrupted when compressed and some values were lost.
- Missing at Random (MAR): Missing values are related to the other observed variables.
 - E.g. People with higher income may to not answer how much taxes they pay.
- Missing Not at Random (MNAR): Missing values are related to the values of the variable itself.
 - E.g : People with higher income may refuse to answer how much money they make.

Taxonomy of Imputation methods



Ref: Do we really need imputation in AutoML predictive modeling? George Paterakis et al. 2023

Mean / Mode Imputation

- Mean Imputation :
 - Used for numeric features that have missing values.
 - Replace missing values with the mean value of the feature.
- Mode Imputation :
 - Used for categorical features that have missing values
 - Replace missing values with most frequent feature value.

X1	X2	Υ
60	'NO'	10
80	'YES'	15
_	'YES'	10
100	-	15



X1	X2	Y
60	'NO'	10
80	'YES'	15
80	'YES'	10
100	'YES'	15

MissForest

Iterative imputation based on Random Forest.

- First the missing values are imputed by mean/mode.
- Then for each feature with missing values, we train a RF on the other features and predict the missing values using the trained RF.
- Continue iteratively using the last imputed dataset till convergence.



Mark missing values as Predict

Use model to generate prediction for missing value

SoftImpute

SoftImpute is an iterative method utilizing a rank-restricted SVD.

- Missing values are zero-imputed
- In each iteration a rank restricted SVD is applied, then the data are projected using the calculated matrices to the original dimensions.
- Continue iteratively using the last imputed dataset till convergence.

Probabilistic PCA

Probabilistic PCA is an iterative method utilizing a generalized PCA.

- Missing values are zero imputed
- In each iteration, PPCA projects data in a lower dimension and reconstructs the data using the learned parameters.
- Continue iteratively using the last imputed dataset.

PPCA assumptions:

Linear generative model: $y_d = \sum_{k=1}^{\infty} \Lambda_{dk} \; x_k + \epsilon_d$

- x_k are independent $\mathcal{N}(0,1)$ Gaussian factors
- ullet ϵ_d are independent $\mathcal{N}(0,\sigma^2)$ Gaussian noise
- $\bullet K < D$

PPCA is factor analysis with isotropic noise: $\Psi = \sigma^2 I$

Denoise Autoencoder

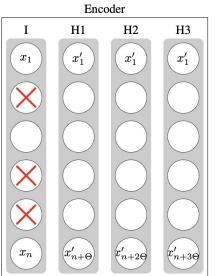
Denoising autoencoders is a neural network that contains an encoder and a decoder.

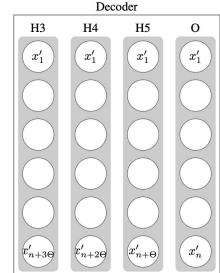
- First it does an initial imputation using mean/mode.
- Then it corrupts the input data by setting a % input of data equal to 0.
 (Dropout-Layer)
- It sequentially it maps data to a higher dimensional space. (Encoder)
- Then it sequentially maps the data to a lower dimensional space till it reaches the original dimension. (Decoder)

Overview of DAE.

We start with an initial n dimensional input, then at each successive hidden layer, we add Θ nodes. Then the decoder maps data to $-\Theta$ dimension

sequentially.





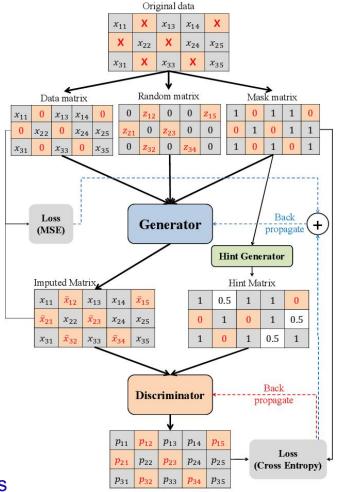
REF: MIDA: Multiple Imputation using Denoising Autoencoders

GAIN

GAIN is a generalization of GAN for the purpose of missing data imputation.

Generator : Tries to accurately impute missing data.

Discriminator: Predict which data are observed and which are imputed given a hint matrix.



Estimated mask matrix

REF: Missing Data Imputation using Generative Adversarial Nets

Missing Indicator

- Missing Indicator Method:
 - Impute missing values with a method.
 - Create a new variable for every feature with missing values.
 - The new variable takes value 1 if value is missing, 0 if not missing.

X1	Υ		X1	X1R	Υ
60	10		60	0	10
80	15		80	0	15
-	10	·	80	1	10
100	15		100	0	15

Hyper-parameters

Method	Hyper Parameter	Values	
MM	-	-	
MissForest	max_depth	10, 20	
SoftImpute	Variance explained	50%, 70%, 90%	
PPCA			
DAE	Dropout	0.25, 0.4, 0.5	
	theta	5, 7, 10	
GAIN	hint_rate	0.5, 0.9	
GAIN	alpha	0.1, 1, 10	