Building a Reproducible Machine Learning Pipeline



What is reproducibility in Machine Learning?

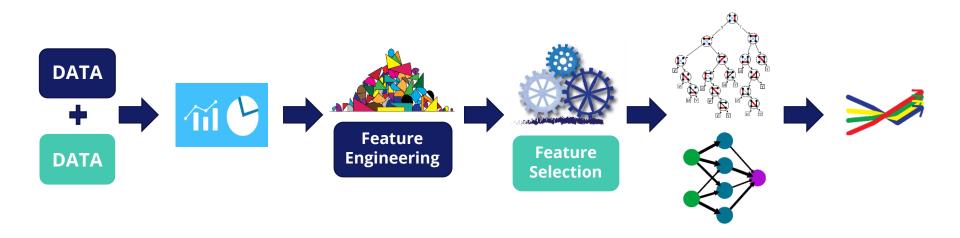


consistent, imitable,
duplicable, duplicatable,
 repeatable



Reproducibility is the ability to duplicate a machine learning model exactly, such that given the same raw data as input, both models return the same output.

Machine Learning Pipeline: Overview



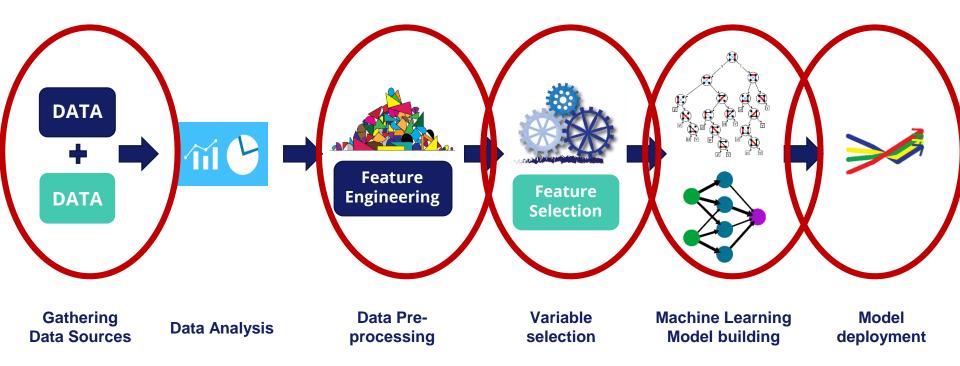
Gathering Data Sources

Data Analysis

Data Preprocessing Variable selection

Machine Learning Model building Model deployment

Machine Learning Pipeline: Production



Reproducibility during data gathering





DATA

Gathering Data Sources

Data can be the most difficult challenge to ensure reproducibility

- Problems occur if the training dataset can't be reproduced at a later stage
- ➤ For example, the databases are constantly updated and overwritten, therefore values present at a certain time point differ from values later on.
- ➤ Order of data during data loading is random, for example when retrieving the rows with SQL.

- Save a snapshot of training data (either the actual data, or a reference to a storage location such as AWS S3
 - √ Good if the data is not pulled from too many different sources
 - Potential conflict with GDPR
- Design data sources with accurate timestamps, so that a view of the data at any point in time can be retrieved
 - ✓ Ideal situation
 - If not in house already, it requires a big effort to re-design the data sources

Reproducibility during feature creation

Lack of reproducibility may arise from:



Feature Engineering

Data Preprocessing

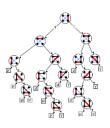
- Replacing missing data with random extracted values
- Removing labels based on percentages of observations
- Calculating statistical values like the mean to use for missing value replacement
- More complex equations to extract features, e.g., aggregating over time

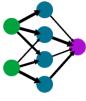
- Code on how a feature is generated should be tracked under version control and published with auto-incremented or timestamp hashed versions.
- ❖ Many of the parameters extracted for feature engineering depend on the data used for training → ensure data is reproducible
- If replacing by extracting random samples, always set a seed

Reproducibility during model building









- Record the order of the features
- Record applied feature transformations, e.g., standarisation
- Record hyperparameters
- For models that require an element of randomness to be trained (decision trees, neural networks, gradient descents), always set a seed.
- If the final model is a stack of models, record the structure of the ensemble.

Reproducibility during model deployment: Software environment and implementation



- For full reproducibility, the software versions should match exactly applications should list all third party library dependencies and their versions.
- Use a container and track its specifications, such as image version (which will include important information such as operating system version)
- Research, develop and deploy utilising the same language, e.g., python
- ❖ Prior to building the model, understand how the model will be integrated in production —how the model will be consumed-, so you can make sure the way it was designed can be fully integrated
 - Examples of partial deployment include, some data not being available at the time of consuming the model live
 - Filters in place do not allow a certain cohort of data to be seen by the model

Building a Reproducible Machine Learning Pipeline: Additional resources

- Building a Reproducible Machine Learning Pipeline
- Introducing FBLearner Flow: Facebook's AI backbone
- Scaling Machine Learning as a service: Uber's pipeline
- A systems perspective to reproducibility in Production Machine Learning
- Hidden technical depth in machine learning systems