ISSUES AND CHALLENGES IN ML ANALYSIS

Tengku Muhammad Hanis Bin Tengku Mokhtar

February 12, 2026

About me

Senior Lecturer
at **UniSZA**

Background

- PhD (Public Health Epidemiology) from USM, 2024
- MSc (Medical Statistics) from USM, 2019
- MBBCh from Al-Azhar University, 2015

Interest:

- Medical statistics, meta-analysis, bibliometrics
- Machine learning and deep learning application in medical sciences
- Application of R on health/medical data

Contact me:

- Email: tengkuhanismokhtar@gmail.com
  tengkuhanismokhtar@unisza.edu.my
- Website: https://tengkuhanis.netlify.app/
  https://jomresearch.netlify.app/

Material

https://github.com/tengku-hanis/applied_ml_seberangjaya.git

Content

Data size

- Generally the bigger the data, the better the model perform
- There are a few sample size calculation available such as using AUC
- However, these methods mostly not appropriate for model training and development - do not take into account the complexity of the algorithms, number of features, etc (personal opinion)
- The idea of sample size in statistical analysis is to have enough power to detect the significant difference - for example, in AUC to detect the difference between AUC of 0.5 (random guessing) and the hypothesized AUC
- These methods are appropriate:
  - As a rough guideline
  - Validating a pre-trained model

Data leakage

- Data leakage occurs when information outside of the training dataset is used to train the ML model
- Example:
  - Train-test contamination: mean imputation use the whole dataset instead of the training dataset
  - Target leakage:
    - Include predictors that are not available at the time of prediction
    - Include the diagnostic information when the model supposed to be a screening model

Curse of dimensionality

- As the number of features (dimensions) increases, the volume of the space grows exponentially, making data points sparse
- This sparsity
  - Makes it difficult for algorithms to find meaningful patterns
  - Increase computational costs
  - Reducing overall performance - models are more likely to overfit because they capture noise instead of the underlying pattern in the data
- Solution:
  - Feature selection
  - Use dimension reduction techniques - PCA, UMAP, t-SNE, etc

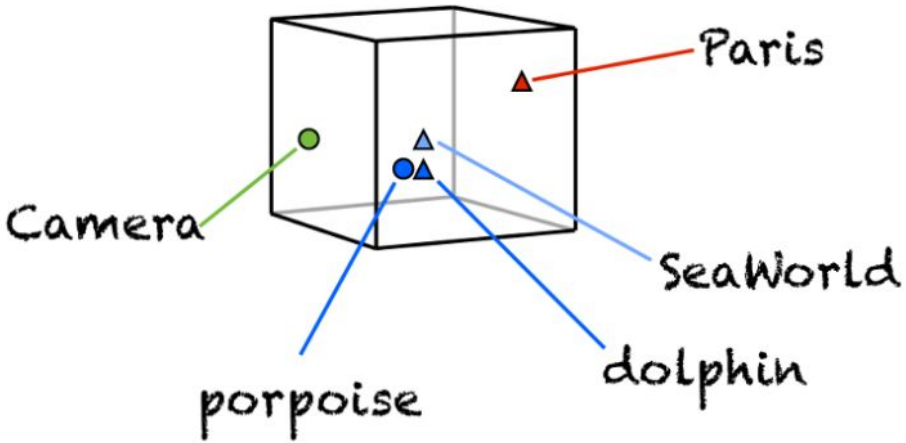
Missing data

- Data should representative of the prediction task
- Missing data may compromise the data representativeness
- There 3 types of missing data mechanisms:
  - Missing completely at random (MCAR):
    - Data missing due to chance
    - Eg: some of the medical records loss due to flooding
  - Missing at random (MAR):
    - Data missing related to the observed variable
    - The missingness can explained by other variable
    - Eg: blood pressure info is missing due to a very big biceps (the clinic only has small to medium cuff)

    - Missing not at random (MNAR);
        - Data missing due to unobserved variable
        - Eg: salary info is missing for people with high income as they feel insecure to disclose their salary
- Basically, only MCAR does affect the data representativeness
- The most effective solution is to take extra measures to avoid missing data (especially MNAR type)
- The ML field is not well developed in this issue to resolve it compared to the conventional statistical analysis field:
    - ML field is more algorithmic or applied approach rather than theoretical one and more focus on prediction rather than inference

Sparse category

- Also known as high cardinality or rare category problem
- The effect of having a sparse category:
  - May lead to overfitting - the ML model might memorise the rare category as there is not enough data to learn from
  - Dimensionality explosion and slow model training process - if we apply one-hot encoding and we have many sparse categories
  - The “unseen” problem - if a sparse category appear only in the test dataset
- Solution:
  - Grouping/binning - combine all sparse category into one group, “others”
  - Embeddings - map categorical variables into a new dimensional space


Paris
Camera
SeaWorld
dolphin
porpoise

Scaling

- Two most common methods:
  - Min-max normalisation

$$x' = \frac{x - \mu}{\max(x) - \min(x)}$$

  - Z-score normalisation (standardisation)

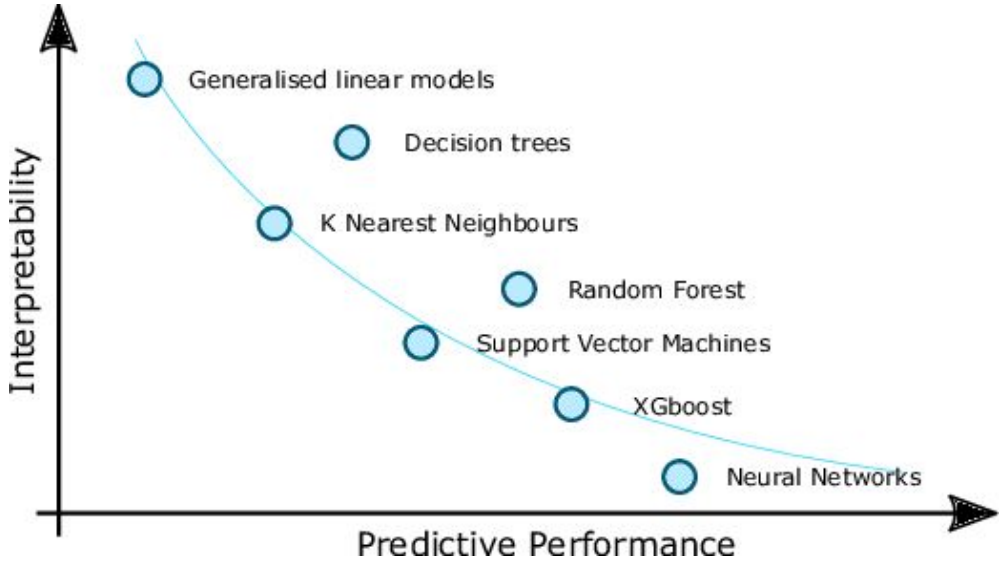
$$z = \frac{x - \mu}{\sigma}$$

$\mu =$ Mean
$\sigma =$ Standard Deviation

- Always scale after splitting the data
- Scaling may help with faster convergence and model performance
- However, not all model benefit from the scaling process:
    - Does not benefit - tree-based models (decision tree, random forest, XGBoost, LightGBM)
    - Benefit - distance-based models (k-NN, k-means, SVM), gradient descent-based model (linear/logistic regression, neural network)
    - More info - refer to tidymodels book

Interpretable ML

- Also known as explainable machine learning
- The is always an inverse relationship between model complexity and interpretability



- There are 2 types of ML model:
  - Glass/white box model:
    - ML models that we can understand the structure and their internal working
    - Decision tree, linear regression, etc
  - Black box model:
    - ML models that are hard/difficult to understand or follow how it reach the prediction
    - Random forest, XGBoost, deep learning, etc

- Some differentiate the terms:
  - Interpretable:
    - A model is considered interpretable if we can understand the internal structure of the model (ie: glass box model)
  - Explainable:
    - A model is explainable when the model itself is “black box”
- There are 2 types:
  - Model agnostic approach:
    - An approach that is universal and can be applied to ML models
  - Model specific approach:
    - An approach that is specific to certain models

- Can also classified as:
  - Global explainer:
    - Explain the behaviour of the model as a whole
  - Individual explainer
    - Explain the behaviour of the model at the specific instances
- Some of the packages that work well with tidymodels ecosystem:
  - lime
  - vip
  - Dalex and DALEXtra (personal recommendation)
  - shapper

- Example of interpretable ML approaches:

Model agnostic + global explainer	**Model specific + global explainer**
- Permutation-based variable importance	- Tree-based variable importance
Model agnostic + individual explainer	**Model specific + individual explainer**
- LIME - Local Interpretable Model-agnostic Explanations - SHAP - Shapley Additive Explanation	- LRP - Layer-wise Relevance Propagation (for DNN)

Deployment

- There are 2 main approaches (that I know of):
  - Plumber (API) and vetiver (version control)
    - Turn R-based ML model into a URL that other program can send data and get prediction
  - Shiny app - example

Suggested readings/references

- Kuhn, M., & Silge, J. (2022). Tidy modeling with R: A framework for modeling in the tidyverse. " O'Reilly Media, Inc.".
- Christoph, M. (2020). Interpretable machine learning: A guide for making black box models explainable.
- Biecek, P., & Burzykowski, T. (2021). Explanatory model analysis: explore, explain, and examine predictive models. Chapman and Hall/CRC.

Any question?

https://tengkuhanis.netlify.app/
https://jomresearch.netlify.app/