Advanced Data Analysis with Python

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Resources for this class

- McGill lecture on Empirical Risk Minimization
- Google Developers Machine Learning Class Course
- McGill lectures on Feature Engineering

Questions about last week's topic

Machine Learning Workflows

From statistics to machine learning

- We studied the **core statistical methods** of data analysis: regression, classification, times series, ...
- Statistics and machine learning **partially overlap**

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- We studied the **core statistical methods** of data analysis: regression, classification, times series, ...
- Statistics and machine learning **partially overlap**
- ML: more focus on **predictions**, statistics: more focus on **inference and patterns interpretation**

- How do we build a machine learning workflow?

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- Where is the shift between statistics and machine learning?

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- Where is the shift between statistics and machine learning?
- When do we need machine learning?

What is machine learning

Definition (Machine Learning)

Machine learning (ML) is a field of study in artificial intelligence concerned with the development and study of statistical algorithms that can **learn from data and generalise to unseen data**, and thus perform tasks without explicit instructions.

Source: Wikipedia

Learning Paradigms

- **Supervised Learning**: an algorithm maps input to output based on example input-output pairs (**labeled data**).
- **Unsupervised Learning**: an algorithm learns patterns from **unlabeled data**.

Supervised Learning

Let D be a dataset of n observations:

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

- $x_i \in \mathbb{R}^p$ — feature vector for observation i
- $y_i \in \mathcal{Y}$ — label (continuous for regression, categorical for classification)

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ML formulation: Learn a function

$$f_\theta : \mathbb{R}^p \to \mathcal{Y}$$

that maps features to labels.

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ML formulation: Discover structure or patterns in the data, such as clusters or low-dimensional representations.

ML model workflow

1. Data collection

ML model workflow

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2. Exploratory data analysis and model selection

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3. Data cleaning

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Feature Engineering

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It includes:

- Target transformations
- **Feature extraction**
- Feature encoding

In this lecture, we will talk about feature extraction. Feature extraction and encoding are more useful for more complex types of models (e.g. neural networks).

Binning

- **Binning** consists of converting a continuous numerical feature into discrete "bins" or intervals, where each bin represents a **range**.

Log Transform

- Takes a numeric feature x and replaces it with $log(x)$
  - Careful: can only work **on positive values!**

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    - Careful: can only work **on positive values!**
- Useful to:
    - Reduce skewness
    - Handle large ranges
    - Reduce effect of outliers

Scaling: Normalization

Normalization involves scaling all values in a fixed range between 0 and 1:

$$x' = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$

- **Scaling** is useful for comparing variables that are in a very different range, such as **age** and **income**
- Effect of **outliers** increases: handle them before!

Scaling: Standardization

Standardization scales the values while taking into account standard deviation:

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

- **Reduces** effect of **outliers**

Other feature engineering techniques

- We handled in the past lectures some feature engineering techniques, such as:
  - Outlier detection (with boxplots)
  - Dataframe grouping and splitting
- Several other techniques exist, also more advanced ones (BagOfWords, Principal Component Analysis, clustering...)

Data handling in ML

Data

- Golden rule: **garbage in, garbage out**
- Some data quality standards to always check for:
  - Missing values
  - Missing features (e.g., the demographics info for the patients are not fully present)
  - Duplicates
  - Imbalanced datasets
- One main question: **Do I have the necessary data to answer my research question?**

Data splitting

- Core concept of ML: **data splitting**
- `train` and `test` set; eventually **evaluation** set

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- Core concept of ML: **data splitting**
- `train` and `test` set; eventually **evaluation** set
- **Why splitting?**
  - Allows you to **test the model on unseen data**
  - Prevents overfitting
  - Ensures generalization

Usual splits

- `train`: the model is **trained** on the training set
- `test`: the model is tested on the **test set**, which consists of unseen data
- `eval`: testing **during training** for hyperparameter finetuning and other adjustements

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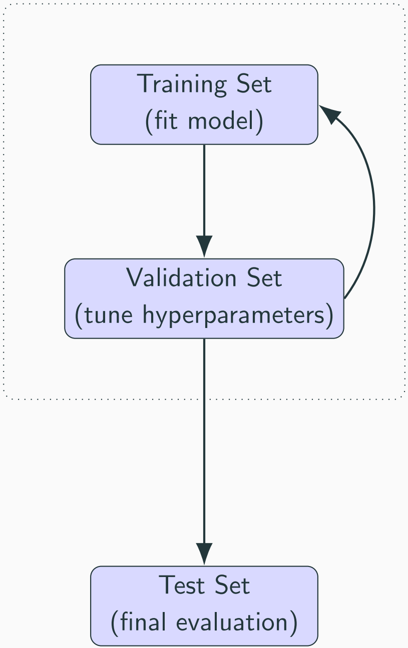
Repeatedly testing the model on the test set to adjust parameters can lead to the model **memorizing patterns from the test set** and thus to misleading results, hence the necessity of an **evaluation set**.


Training Set
(fit model)
Validation Set
(tune hyperparameters)
Test Set
(final evaluation)

Common splits

- 70% train, 15% test, 15% eval
- 80% train, 10% test, 10% eval
- The best proportion is very **dataset-dependent**: you will have to **experiment with the data** to find it.

Imbalanced datasets

Example of **classification** problem:

- Dataset is **imbalanced** if the ratio of different classes presents a strong misproportion.

Consequences

- The model does not learn the **features of each class**
- The model does not learn the **class distribution**

Stratified split and k-fold cross-validation

- Stratified split (available in `sklearn`): to respect a specific balance in the data split
- K-fold cross-validation: if the dataset is very small, chances are that the test samples will be imbalanced. You can avoid this by:
  - **dividing the dataset into K equal-sized folds**
  - For each iteration, training on $K-1$ folds and testing on the remaining one

Downsampling and Upweighting

If the dataset is strongly imbalanced, these methods will not be effective. In that case, you can proceed with:

1. Step 1: **downsampling**
2. Step 2: **upweighting**.

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- Artificially reduce the majority class
- Consequence: the minority class will be **represented enough**

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With this method, you introduce a **prediction bias** (careful: this is different from the **bias term** that we talked about in the previous lectures!

Upweighting

- To deal with the **prediction bias**, the **errors** need to have a bigger weight
- **You must "upweight" the majority classes by the factor to which you downsampled**
- Meaning: when the model mistakenly predicts the majority class, treat the **loss** as if it were 25 errors (multiply the regular loss by 25).

Imbalanced datasets: caveat

- While **class imbalance** is a very specific problem of **classification approaches**, the data distribution is essential to the **data quality**
- Therefore: **imbalanced datasets** are always an issue, not only in classification
- Examples:
  - Biases in linear regression: e.g. wage data: your test set contains many **high salaries**, but we know that this is only the case for a few people
  - Therefore: importance of accurate **variable selection** and **data splitting**.

Model validation and tuning

Hyperparameters

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- Not all models have hyperparameters; usually for more complex models, e.g. neural networks
- **OLS regression**: normally no hyperparameter; if regulated, it can have hyperparameters

Loss Function

Definition

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- Quantifies **how wrong the model is**
- Goal: **minimize the loss**
- We discussed **evaluation metrics** for each presented method - they are useful to **computing the loss** (attention: several ways of doing that!)

Risk Minimization

Definition

The **risk** of a model is the **expected loss**.

$$R(f) := \mathbb{E}_{x,y}[L(y, f(x))] = \int L(y, f(x))\, dP_{x,y}$$

Where:

- $L(y, f(x))$ is the loss
- $P_{x,y}$ is the data distribution

Usually, we do not have access to the **real distribution**, but to a **training set and test set** that **represent the data**. (Remember the population vs sample differentiation in statistics!)

- Therefore: one possible methos is **empirical risk minimization**

Overfitting

Definition

We speak of **overfitting** when the models learns the training set so closely that it fails to **generalize** on unseen data.

- Real-world problem! In **applicative settings**, you need your model to be able to predict on new data as accurately as possible.

Underfitting

Definition

An **underfitting** model fails to performs well even on the training data.

Overfitting and underfitting example

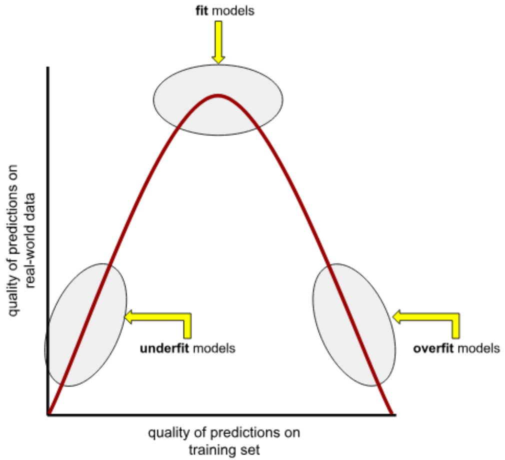

Figure 14. *Underfit, fit, and overfit models.*

Source: Google Developers Crash Course on ML.

How do you detect overfitting?

- Indicator: **loss function**
- Plot the loss function; a plot with several loss function is called the **generalization plot**
- If the model **overfits**, the loss curve is good at first, and then **diverges**

Regularization

- The idea behind **regularization** is to minimize both **loss** and **complexity**, thus fitting the data **as well as possible** but also **as simply as possible**.

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- Two base methods:
  - **L1 regularization (used for LASSO)**: adds a penalty based on the **absolute value** of coefficients.
  - **L2 regularization (used for ridge regression)**: adds a penalty based on the **square** of the coefficients.

L1 Regularization (LASSO)

Lasso adds an L_1 penalty:

$$\text{Loss} = \text{MSE} + \lambda \sum_{i=1}^{n} |w_i|$$

Characteristics:

- w_i are the **weights** (=coefficients)
- Produces sparse models (many $\beta_j = 0$)
- Performs feature selection
- Unstable when predictors are highly correlated

L2 Regularization (RIDGE)

Ridge adds an L_2 penalty on coefficient magnitude.

$$\text{Loss} = \text{MSE} + \lambda \sum_{i=1}^{n} w_i^2$$

Effects:

- No coefficients become exactly zero (no feature elimination)
- Works well with correlated predictors

Common uses of ridge and lasso

- **Lasso**:
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Common uses of ridge and lasso

- **Lasso**:
  - Feature selection
  - Some predictors have a way bigger impact than others
- **Ridge**:
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  - You do not want to **zero out** any predictor

Caveats:

- Those are not the only existing regularization techniques, but the only ones we will hand here
- This is an **experimental** process, so these regularization techniques might not always be beneficial
- Always prioritize **interpretability** of your model.

The Big Picture of this course

How does everything fit together?

- This course mixed a **statistical approach** to **lab sessions**
- Here, we are introducing **ML concepts** to ease the shift from statistics to ML

- **Exploratory data analysis** has a descriptive intent, and is often the first step to assess **which model to use** and switch to a **predictive setting**
- **Linear regression and classification** are the basis of ML, the simplest models, and essential to understanding **more complex models**
- **Time series** are a more complex statistical topic; they fit under ML if regarded in their predictive aspects, but beware of the added complexity of time measurement
  - Example: if **splitting data**, the different time of the data must be taken into account
- **Causal Inference** expands traditional ML to include **causality** - but we saw its strong relation to **linear regression**

Questions?

Final project guidelines

- The code needs to be **on GitHub** (you can create a private repository and add me as a contributor, meaning **I will receive an email giving me access to your code**)
- Do this at the end, when you finished the modifications
- The paper needs to **contain the reference to the repository**. You will **upload it on Moodle** (only one upload per group!)

Final project guidelines

- **Requirement: predictive step**
- While a focus on EDA and graph-based representations is perfectly fine, the project **must contain at least one of the models we studied**

Deadline on **December 20**!