1 Introduction

High-quality produced chocolate is indispensable in the production of all kinds of confectionery. In order to produce these high-quality products, the chocolate itself need to be tempered in a defined manner. This tempering process is the very first step in every production. Customers as well as manufacturers announce clear requirements regarding the quality of the choclate. The requirements are as follows:

- **Excellent taste:** Taste is the primary selling point. An exceptional flavor is therefore of high importance for the success of a chocolate product.
- **Customer demands:** Demands are not focused on the taste, but also on the appearence and texture of the chocolate represents essential features of high-quality chocolate.
- **Reputation and trust:** A consistent quality of chocolate enhances the reputation and customer trust in the company.
- **Processing efficiency:** In context of an industrial production process, flow characteristics, a clean break, a glossy surface and easy release after a molding process are crucial parameters. Such parameters can only be achieved by a high-quality chocolate mass and a stable tempering.

To meet these demands, the company Sollich KG from Bad Salzuflen has been manufacturing high-quality machinery for processing confectionery for over 100 years. Specifically, they produce tempering machines for the pre-processing of chocolate mass. Only through stable pre-tempering a crispy chocolate with good flow properties and a distinctive shine is achieved. The correct tempering increases shelf life and prevents the formation of fat bloom on the end product.

The process has been mastered steadily for decades. However, for sustainable production, it is important to avoid unnecessary hardware, in order to lower energy consumption, implementation work and costs. Therefore, Sollich is interested in utilizing methods from the field of artificial intelligence (e.g. machine learning, stochastic processes or optimization). This is ensured through modern sensors and continuous data collection in the machines of the newest generation. Current endeavors in the preliminary development of new machine generations aim to implement the use of soft sensors for process control. Soft sensors will not only save steel parts in the tempering section, but also reduce complexity of the electrical wiring, save electrical parts like IO cards and therefore time. To reach this goal a precision of at least 0.1 °C has to be assured.

2 Task

Train a model to estimate each target variable and build a python script called: "run.py" which is able to calculate the regression for a given (as path to folder) set of input files in the parquet format.

Tempering chocolate simply means melting the chocolate while controlling its temperature curve. This technique allows the chocolate to be processed, enabling the productuib of a perfect result for the end product. Sollich's tempering solution addresses this at an industrial level. The chocolate mass is passed through three cooling zones with each zone mixing the chocolate as homogeneously as possible using agitators.

- **Heating Stage:** The purpose of the heating stage is to melt all crystalline structures in the chocolate so that the tempering process can begin.
- **Cooling Stage:** The cooling stage takes on the task of cooling the chocolate according to the optimal cooling curve in a stable manner. Within the chocolate mass, this process infuses seeds of the optimal crystalline structures. When the mass cools down completely in the end product, the seeded crystalline structures ensure that these structures mostly form in the product.
- **Mixing Stage:** The conclusion of tempering involves a mixing stage, primarily aimed at distributing the formed crystalline structures throughout the mass. The temperature used in this stage also ensures that no further crystalline structures are created. Typically, the chocolate is gently heated (depending on the mass) during this phase.

In each of the aforementioned tempering stages, water is used as the medium for tempering. Electric heating elements heat the water and cooling is achieved through a valve at the inlet of the cooling water. This valve is opened for a certain duration (fractions of a second) by the control system allowing cooling water to flow into the system.

3 Dataset

The entire dataset comprises four weeks of production data from the laboratory temper 650B. These data were pre-divided into three datasets. Two days of the week are provided as training data, another day is for evaluation. An additional day is withheld by the jury to conduct the final evaluation (described in chapter 5) using that data.

The data is provided in the 'parquet' format and is named according to the day. Figure 1 illustrates how a parquet file can be read.

The data consists of 68,401 rows per day with each row representing one second of recorded data. The data was recorded from 01:00 AM until 08:00 PM on the same day.

Each dataset includes 13 sensor points as well as the corresponding targets for mass and water.

- **ProzessData_ActData_AB1_Analogs_DX1_MassPressure**
  The pressure that exists within the pipe system when the chocolate mass enters the heating stage. This pressure can change during the tempering

```python
import pandas as pd

# Annahme: Du hast eine Parquet-Datei mit dem Namen 'beispiel.parquet'
parquet_datei = 'beispiel.parquet'

# Daten aus der Parquet-Datei laden
df = pd.read_parquet(parquet_datei)

# Die geladenen Daten anzeigen
print(df)
```

Figure 1: Example to load the provided parquet files as pandas DataFrame.

process, depending on factors such as the viscosity of the chocolate mass, the flow rate, and the operating parameters of the heating stage.

- **ProzessData_ActData_AB1_Analogs_GY1_MassLevelTank**
  The mass level in a tank refers to the measurement of how much chocolate mass is present or stored inside the tank at a given point in time. It indicates the height or volume of the substance within the tank.
- **ProzessData_ActData_AB1_Current_DV1_Scraper**
  Current of the motor driver rotating the tempering column in amperes.
- **ProzessData_ActData_AB1_Speed_DV1_Scraper**
  Frequency of motor driver rotating the tempering
- **ProzessData_ActData_AB1_Current_DW1_RiserPumpFwd**
  Current of the mass transfer pump in amperes. The mass transfer pump moves the material throughout the entire process.
- **ProzessData_ActData_AB1_Speed_DW1_RiserPumpFwd**
  Delivery rate of the conveyor pump in kg/h. The mass conveyor pump moves the material throughout the entire process.
- **ProzessData_ActData_AB1_Temperature_DP1_MassHeatingStage**
  Mass temperature measuring at the heating stage in C°.
- **ProzessData_ActData_AB1_Temperature_DP1_WaterHeatingStage**
  Water temperature measuring at the heating stage in C°.
- **ProzessData_ActData_AB1_Temperature_DQ1_MassCoolingStage**
  Mass temperature measuring at the cooling stage in C°.
- **ProzessData_ActData_AB1_Temperature_DQ1_WaterCoolingStage**
  Water temperature measuring at the cooling stage in C°.
- **ProzessData_ActData_AB1_Temperature_DS1_WaterPipe**
  Temperature of the water from the pipe trace heating.
- **ProzessData_ActData_AB1_Temperature_DU1_WaterTank**
  Watertemperature in the manteling of the tank.

- **ProzessData_ActData_AB1_Temperature_DX1_MassInfeed**
  Mass temperature of the incoming chocolate mass at the beginning of the heating stage.

The regression target variables to estimate:

- **ProzessData_ActData_AB1_Temperature_DR1_MassMixingStage**
  Mass temperature measuring at the mixing stage in C°.

- **ProzessData_ActData_AB1_Temperature_DR1_WaterMixingStage**
  Water temperature measuring at the mixing stage in C°.

4 Submission

For the submission of the group's results, these are the criteria that must be met:

- **Executability**: You should submit a Python script named "run.py". This script should accept a folder path as input (either as an argument or hardcoded within the script). This folder path will contain the evaluation files, which are the same format as the given one, but from different days.

- **Output**: The output of 'run.py' should consist of four files, saved in the same format as the target files, which contian the target variable. Each output file should have a name that clearly corresponds to the input data by using the suffix '_pred'.

- **Completeness**: The script for training the utilized model, as well as the model itself, are part of the submission.

- **Uniqueness**: All results must be placed in a folder named according to the group's name.

5 Evaluation criteria

For the evaluation of the results the jury uses an evaluation dataset, which includes one day from each of the provided weeks. To determine the achieved points for the tasks, standard metrics are not used. The metrics are fundamentally related to the 'Mean Absolute Error' (MAE), so training against the MAE can, in a first approximation, provide good results. However, since the ultimate goal of the entire challenge is to control the system based on the estimated values, it is misleading to consider only the average error. Furthermore, individual strong outliers in regression are not as significant as long-term, persistent average estimation errors, which will lead to significant deviations in control behavior. Therefore, the results are evaluated using the following two metrics:

- **Weighted Absolute Error**: According to a histogram, the following absolute error intervals are evaluated.
  - *[0, 0.05]* (1 point)
  - *(0.05, 0.1]*: (0.5 point)
  - *(0.1, 0.5]*: (0.25 point)
  - > 0.5: (0 point)

  The predicted values are divided into these intervals, and the percentage of intervals in relation to the total length is calculated. The achieved percentage is then multiplied by a factor, and the sum of the points obtained in this metric is calculated. The maximum score of **100** is achieved when all errors are less than 0.05. This metric is related to MAE but evaluates very large outliers differently than MAE does.

- **Error Duration**: As described earlier, individual outliers in the estimated values are not as critical as persistent estimation errors. Therefore, for the second metric, we examine the duration of error blocks. An error block is considered when the absolute error is greater than 0.1. The time intervals are evaluated as follows:
  - *[0, 1]*: The maximum possible intervals are $Y_k/2$, where Y_k corresponds to the number of estimates.
    (0.5 point)
  - *[2, 10]*: The maximum possible intervals are $Y_k/8$, where Y_k corresponds to the number of estimates.
    (0.25 point),
  - > 10*:*
    (0 point)

  For all predicted values, the percentage of values less than 0.1 is calculated. The full point value is derived from this percentage. Weighted points from the time intervals described above are then added to this. The points from a time interval are calculated by determining the maximum possible number of intervals and then finding the ratio of the discovered intervals in the prediction to the maximum possible intervals. The points are then calculated as $100\% - ($*percentage of time intervals*$)$.

Note: All calculated points are rounded down.

Hint: The metrics used can be independently implemented for targeted training.