A World Leading SFI Research Centre

Science Foundation Ireland For what's next

MLGIG Team – Milk Lactose Prediction Data Challenge

Insight SFI RESEARCH CENTRE FOR DATA ANALYTICS

[georgiana.ifrim thach.lenguyen timi.aderinola davide.serramazza] @insight-centre.org

4th International Workshop on Spectroscopy and Chemometrics 2024

Insight Seminar, 15/05/2024

HOST INSTITUTIONS

DCU Ollscoil Chathair Bhaile Átha Cliath Dublin City University · Ollscoil na Gaillimhe University of Galway · UCC University College Cork, Ireland Coláiste na hOllscoile Corcaigh · UCD Dublin

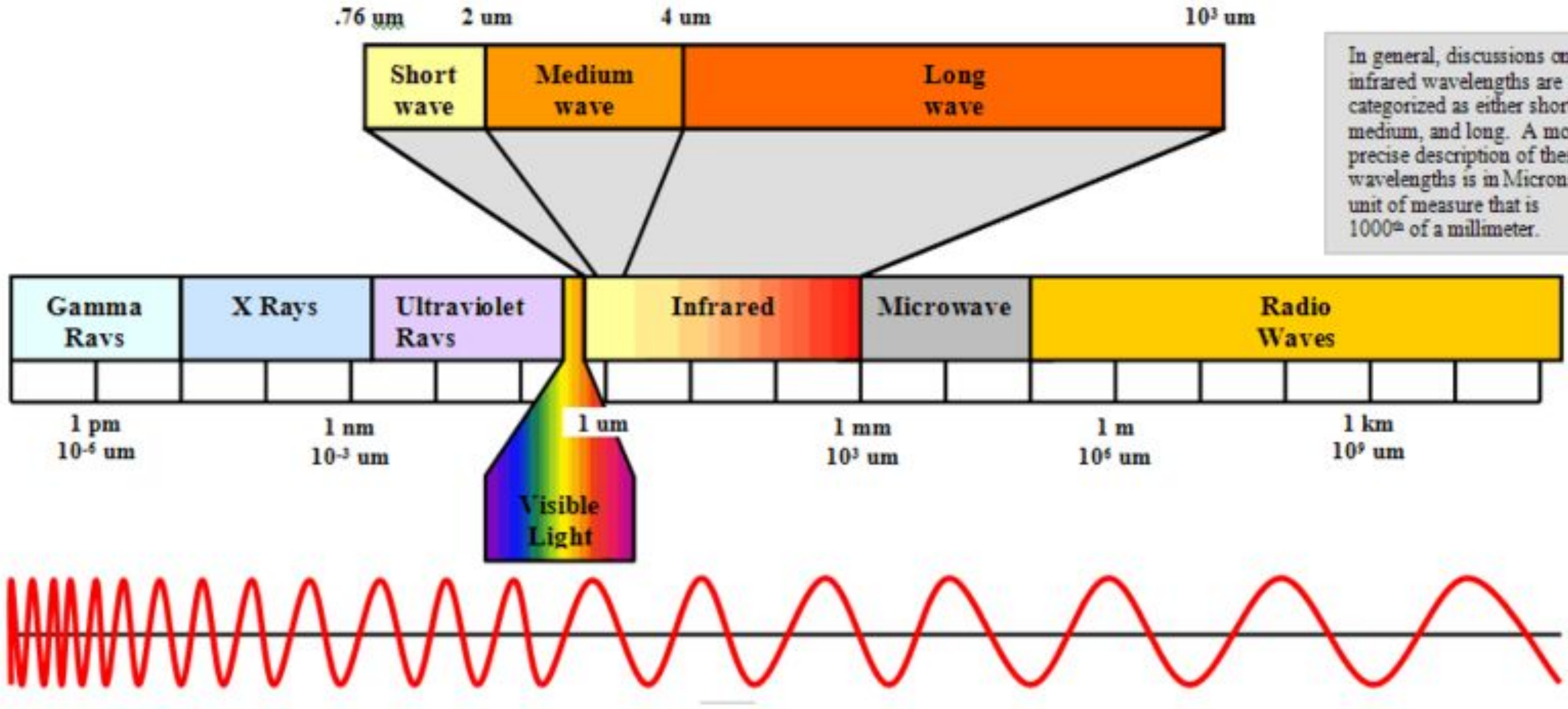
PARTNER INSTITUTIONS

Maynooth University National University of Ireland Maynooth · Tyndall National Institute · Trinity College Dublin Coláiste na Tríonóide, Baile Átha Cliath The University of Dublin · University of Limerick Ollscoil Luimnigh

FUNDED BY:

Ireland's European Structural and Investment Funds Programmes 2014-2020 Co-funded by the Irish Government and the European Union · European Union European Regional Development Fund · Science Foundation Ireland For what's next

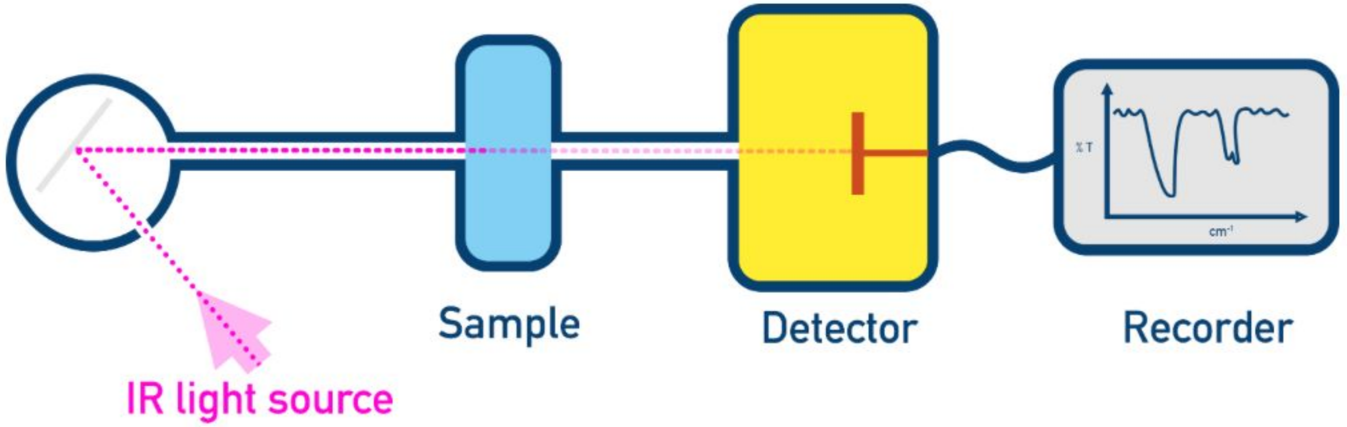
Properties of Light – Infrared Spectrum



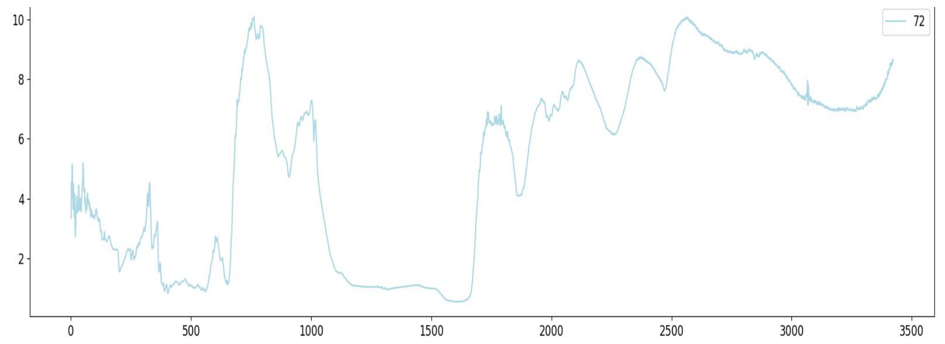
In general, discussions on infrared wavelengths are categorized as either short, medium, and long. A more precise description of these wavelengths is in Microns, a unit of measure that is 1000th of a millimeter.

Insight

Spectroscopy to Analyse Milk Properties



Recorded spectrum for a milk sample



- **Infrared spectroscopy** (IR spectroscopy or vibrational spectroscopy) is the measurement of the **interaction of infrared radiation with matter by absorption,** emission, or reflection.
- Used to study and identify chemical substances or functional groups in solid, liquid, or gaseous forms.
- Commonly employed to **monitor and quantify milk quality parameters**, such as concentrations of fat, protein and **lactose**.

Insight

About MLGIG Team

- **Georgiana** (Assoc Prof@UCD-CS), **Thach** (postdoc Insight@UCD-CS), **Timi** (postdoc Insight@UCD-CS), **Davide** (PhD ML-Labs@UCD-CS)

- Our background is in ML/AI modeling, time series, XAI for time series; no domain expertise in spectroscopy

- **Our code, results and slides are available** (Python Jupyter notebooks):

https://github.com/mlgig/VM-challenge-lactose-prediction-2024

Outline

- Data Understanding and Preparation
- Modeling Approaches
- Results
  - Part 1: Best Predictive Model
  - Part 2: XAI to Improve the Best Predictive Model (Thach)

Data Understanding and Preparation

Data Challenge: Spectral imaging to quantify lactose concentration in dried whole milk

Motivation: need a cost-effective, accurate and robust lactose quantification method

[1] Single-drop technique for lactose prediction in dry milk on metallic surfaces: Comparison of Raman, FT – NIR, and FT – MIR spectral imaging, Caponigro et al, Food Control, 2023

https://www.sciencedirect.com/science/article/pii/S0956713522005448#:~:text=Raman%2C%20FT%2DNIR%2C%20and,%3D%200.98%20mg%2FmL)

Data Understanding and Preparation

- Milk sample used to extract a 3d image (hyperspectral cube).
- Each pixel represented by a spectrum. **Sample = 2d image, pixels on rows and spectrum on columns.**

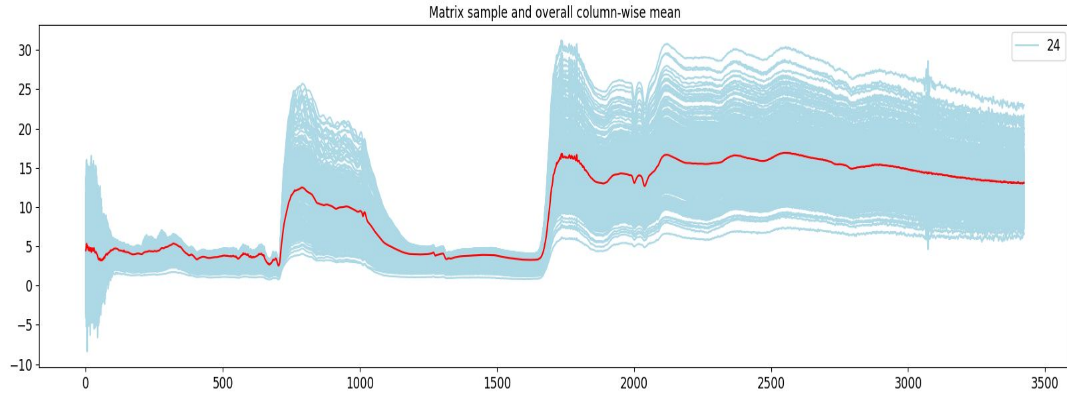
- 64 samples to train (with known targets)
- 8 samples to test (no targets)

- **Target: lactose concentration measured in mg/mL**
- We represent each sample as a matrix with 300 rows and 3424 columns*.

*Subset of pixels for each image (from 112 to 300 pixels). Not all samples have the same number of rows, eg sample14 has 238 rows. We padded the rows with zeros up to 300 rows.

3D image

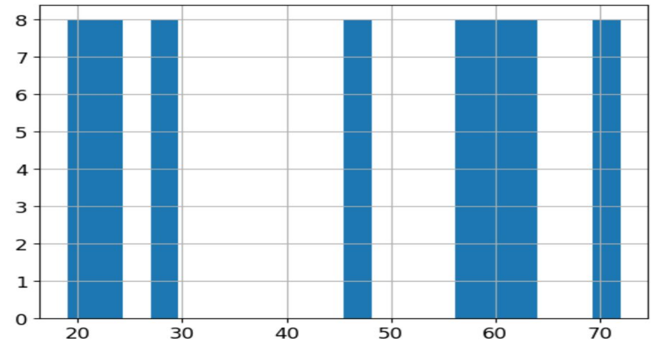
2D image



Data Understanding and Preparation

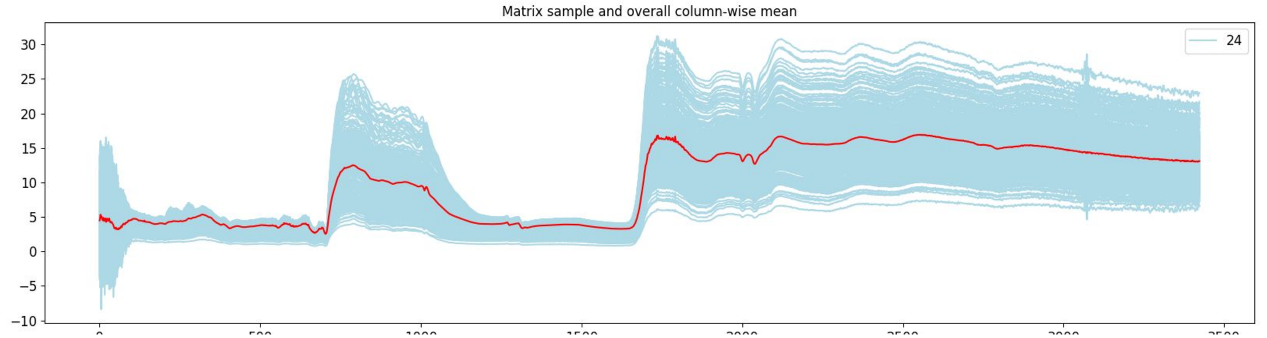
3 groups of train targets: 8 labels x 8 samples

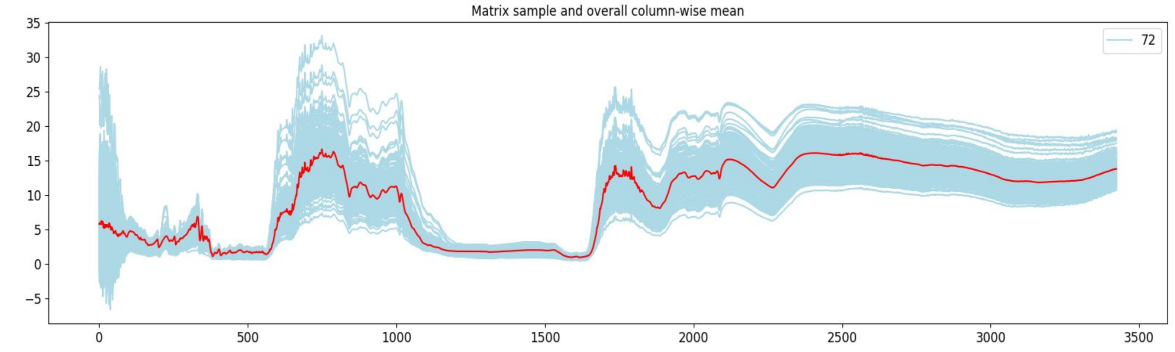
- Low Lactose (19, 24, 29): 24 samples
- Medium Lactose (48): 8 samples
- High Lactose (58, 60, 62, 72): 32 samples

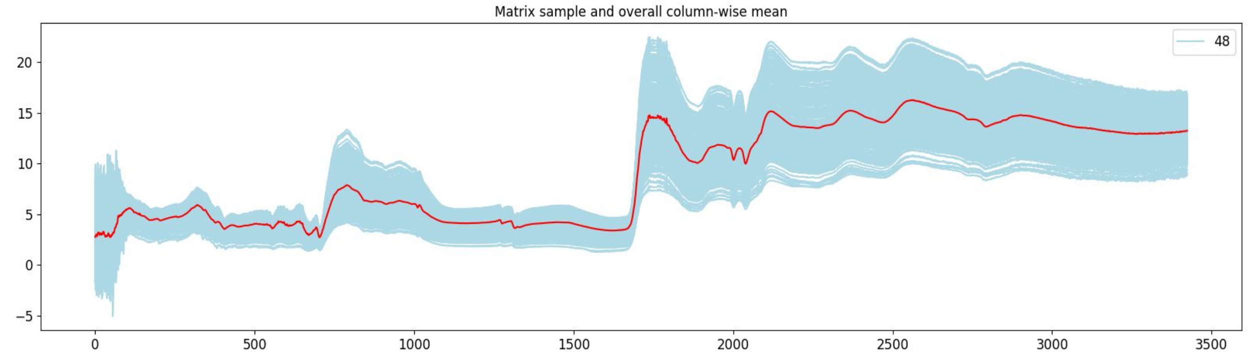


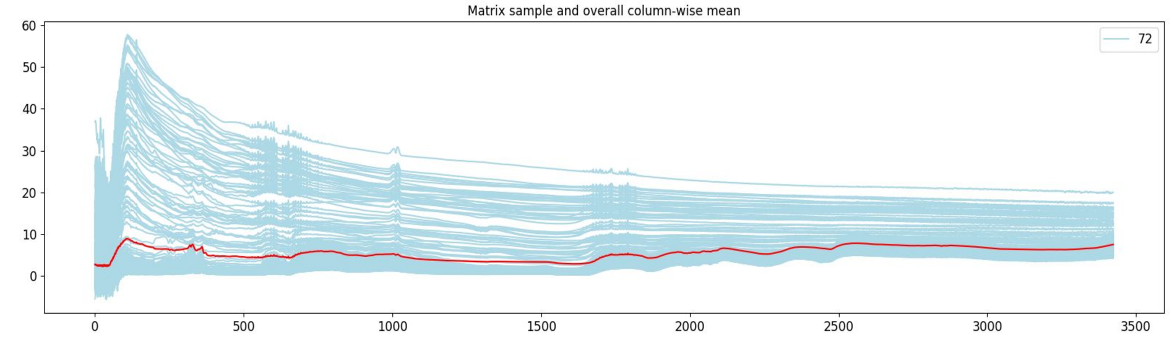
```
train_y.sort_values().value_counts()
```

```
lactose content
19    8
24    8
29    8
48    8
58    8
60    8
62    8
72    8
```



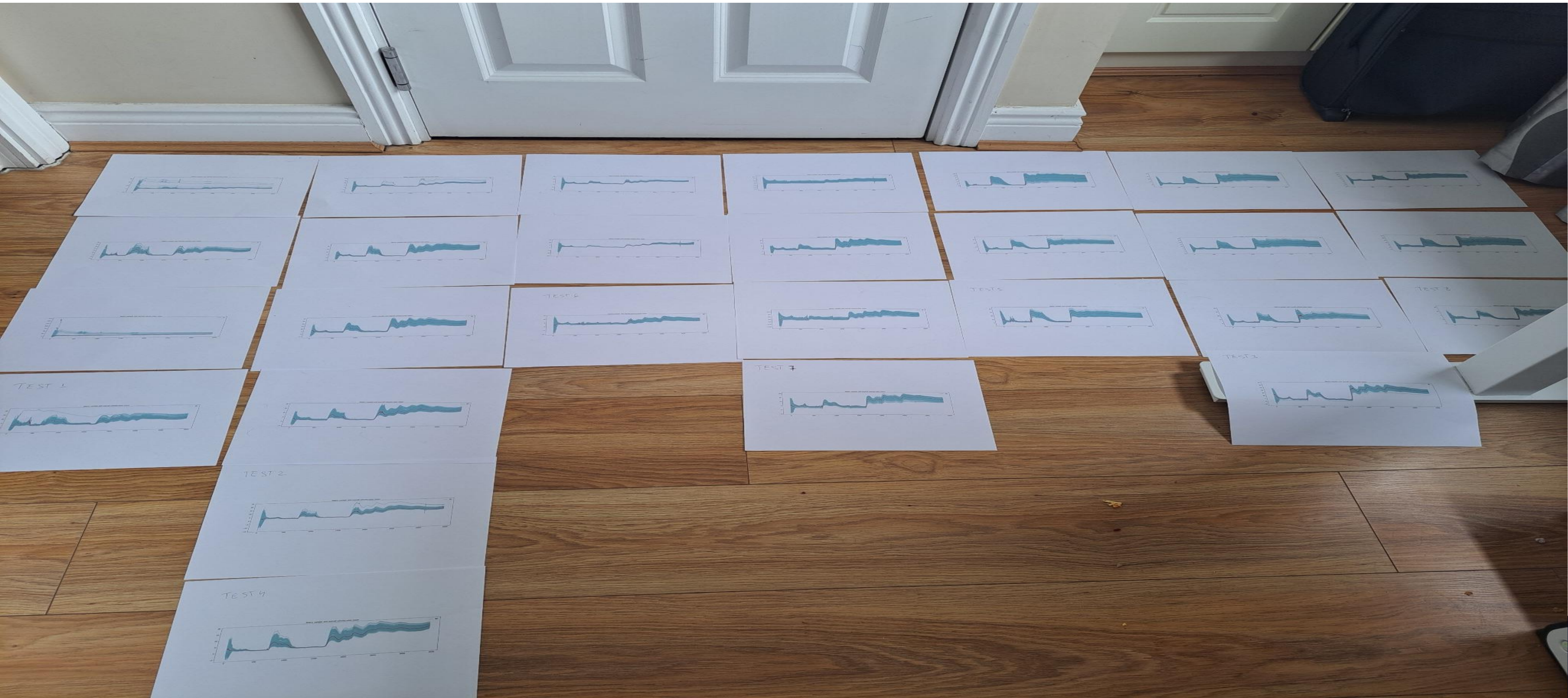






Data Understanding and Preparation

64 samples from 3 groups of lactose concentration (left most in the image is 72, 60/62, 58, 48, 29, 24, 19)



Data Understanding and Preparation

Challenges:

1. **Storage:** Training data is about 700Mb. Can we reduce the data and still get good results?
2. **Noise:** Feature selection: can we remove features that are noisy? Eg variance thresholding, spectrum/column selection or pixel selection?
3. **Outliers:** How to deal with outliers?
4. **Small training set:** Number of samples is very low, only **64 samples to train.** This suggests preferring simpler models to complex DL models.

Modeling Approaches

What methods can we use to work with this data?

1. **Tabular methods:** if we concatenate the rows, each sample is a vector of features (temporal ordering discarded). Each vector will have 300 rows x 3424 columns = **1,027,200 features**. Can use all classic ML methods. Python library numpy, pandas, **sklearn**.

2. **Time series methods**: Each sample is a **time series (ordered features)** with multiple channels/rows. Python library: **aeon**, captum.
    a. Multivariate time series regression (and channel selection methods).
    b. Univariate time series regression (flatten the data to a single row).

3. Deep Learning methods: Models that work well with images; CNN, FCN, Resnet. Python library: **aeon, pytorch.**

Evaluation

- Regression task (numeric target): **RMSE and R2 as evaluation measures** for predictive quality. We keep track of **train+test runtime** to understand accuracy/efficiency tradeoffs.

- Single train/test 75/25 split to check what the model learns (shuffle the data before split), and where possible what are the important features.

- **4-fold Cross Validation (4CV) to compare different algorithms and estimate generalisation ability; <u>model selection based on avgCV-RMSE</u>**

- Select best model using CV -> train best model on the full training set -> predict on test.

- Extra sanity check: Look at predicted targets on test data and consistency across different predictive models Plot each test sample versus predicted target.

Results - Summary

Summary of key findings about modeling, then detailed results.

- Tabular (with row concatenation) is similar to DL methods
  $<_{\text{worse}}$ Multivariate TSR
  $<_{\text{worse}}$ **Univariate TSR (with data flattened to a percentile)**

- DL methods we tested don’t work well wrt RMSE (small data, noise, outliers)
- Data denoising is important for this problem
- **Time series methods work well on this problem**
  - Methods that work in the time domain (interval-based, eg ROCKET, MrSQM-SAX) are better than those working in the frequency domain

Runtime: varies from days to minutes

Results - Summary

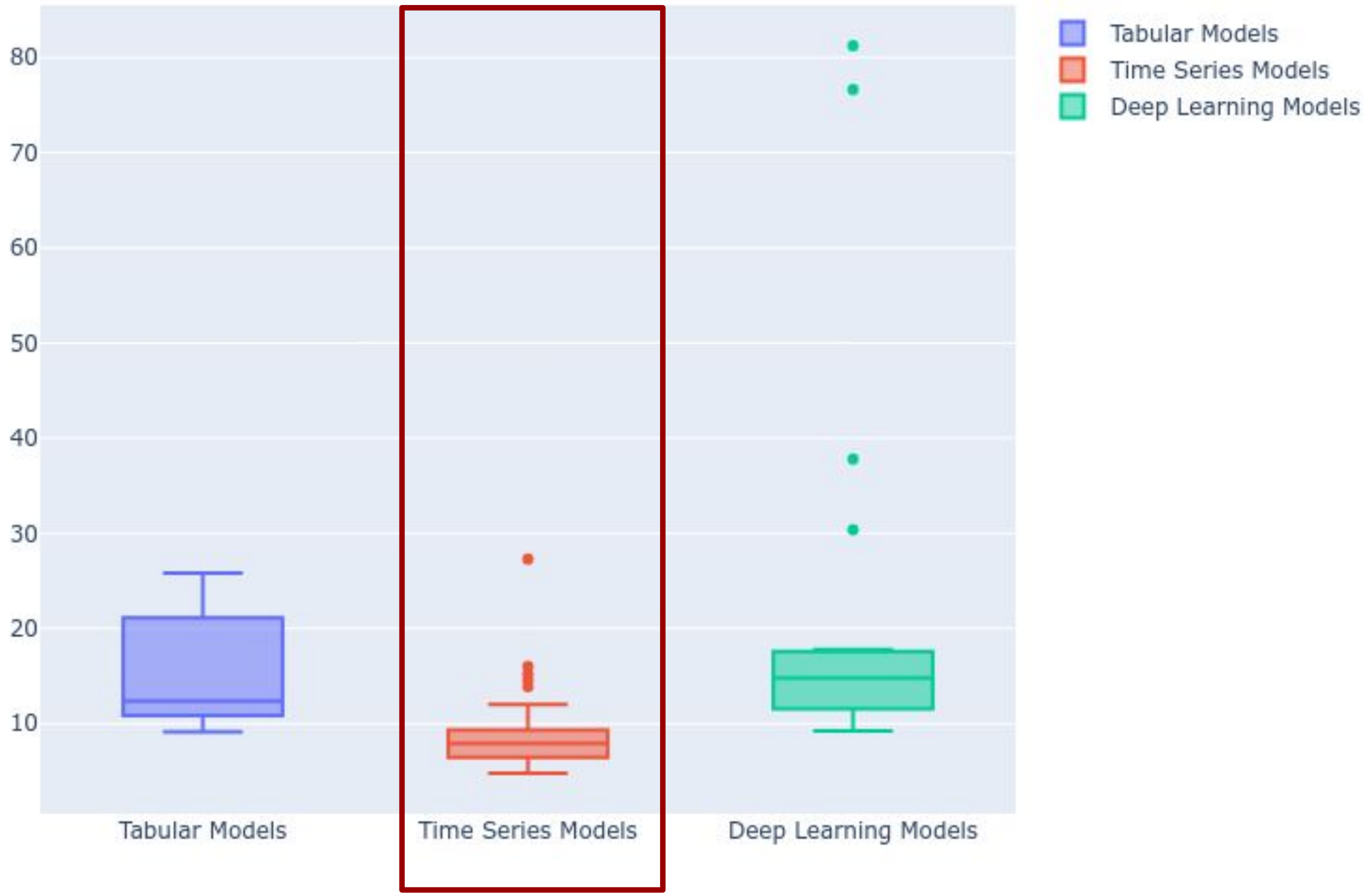
Boxplot of **4CV-RMSE** for models in each group

Tabular Models: Linear Regression, RidgeCV, PLSR, KNN

Time Series: 1NN-DTW, Catch22, DrCIF, Interval Forest, **ROCKET**, MiniROCKET, MultiROCKET, Random Interval, RISE, TSForest, TSFresh

Deep Learning: CNN, FCN, Inception Time, ResNet, TapNet

More detailed results here



Time series group has the best performance on average

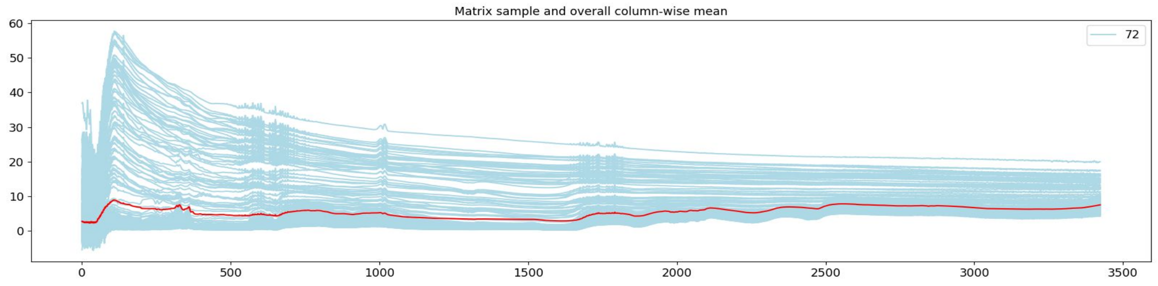
Results - Detailed

Baseline RMSE: 18.62 (for each sample in the training set, predict the average target as computed on the training set)

Method: Tabular **Concatenate all rows/channels**	**4CV avgRMSE**	**Predictions on test samples**
RidgeCV()	19.19	[56.34, 68.44, 42.64, 71.62, 6.39, 49.31, 36.04, 40.94]
KNeighborsRegressor()	13.29	[59.6, 52., 39.4, 60.4, 24., 57.6, 49., 49.6]
PLSRegression(n_components=5)	17.32	[71.23, 59.32, 37.,16, 61.66, 13.47, 50.01, 42.71, 46.31]
Best model: Noise cleaning + KNN Pipeline(StandardScaler()), SelectFromModel(estimator=RidgeCV())), KNeighborsRegressor())])	**12.08**	[61.6, 52, 29.8, 60.4, 26, 52.4, 36, 53.2]

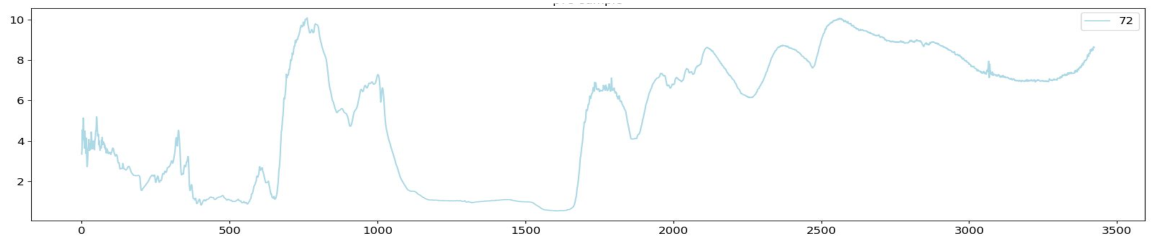
Insight

Results - Detailed



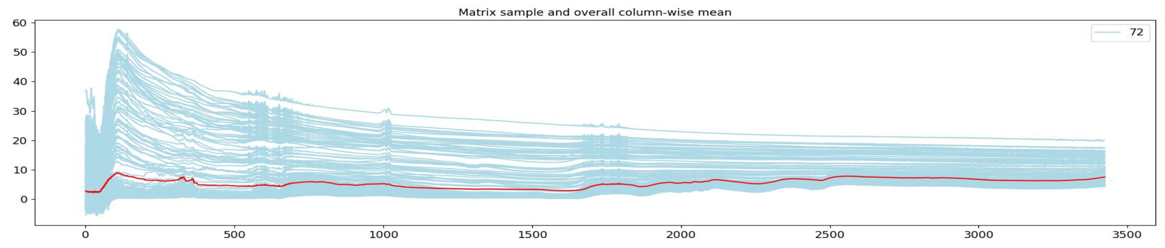
Outliers!

Data flattened to p75 =>



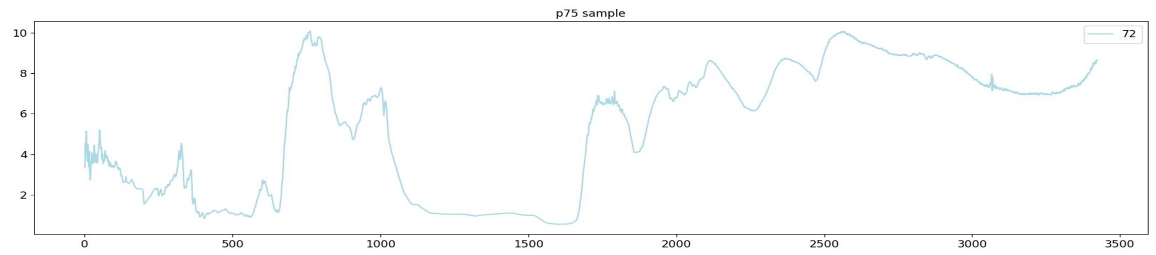
Method: Tabular **Flatten to percentile (p25, p50, p75)**	**4CV avgRMSE**	**Predictions on test**
p25 RidgeCV()	14.32	[64.67, 62.55, 45.26, 66.77, 39.28, 49.76, 38.81, 34.52]
p50 PLSRegression(n_components=10)	9.83	[70.64, 64.9, 43.97, 67.14, 35.91, 42.91, 40.32, 38.49]
Best model: **p75 RidgeCV()**	**9.60**	[71.28, 66.38, 55.84, 63.8, 37.71, 52.86, 48.99, 35.64]

Results



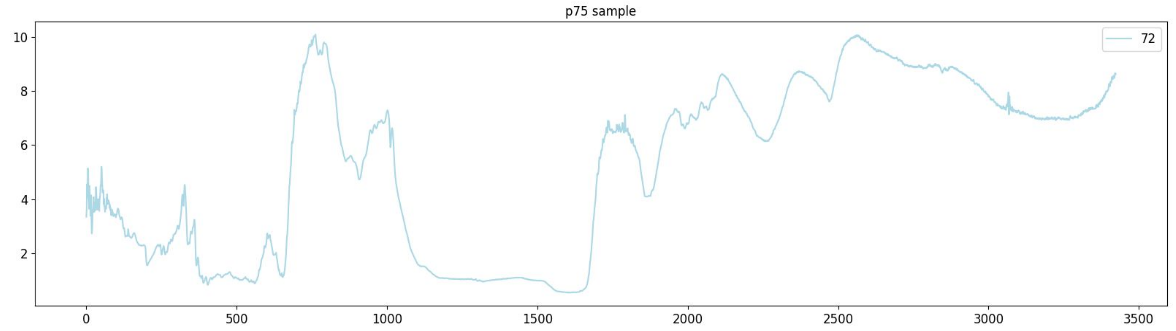
Method: Multivariate Time series	4CV avgRMSE	Predictions on test
All Channels Pipeline(Rocket(random_state=42)), StandardScaler()), SelectFromModel(estimator=RidgeCV())), RidgeCV())])	7.13	[73., 65.12, 41.17, 64.59, 25.79, 46., 46.25, 31.16]
Pipeline(Rocket(random_state=42)), StandardScaler()), SelectFromModel(estimator=RidgeCV())), ExtraTreesRegressor())])	7.00	[71.73, 61.05, 48.51, 61.37, 26.13, 54, 84, 50.46 23.57]
Subset of channels [p25, p50, p75] **Best model: ROCKET + noise cleaning + ExtraTreesRegressor** Pipeline(Rocket(random_state=42)), StandardScaler()), SelectFromModel(estimator=RidgeCV())), ExtraTreesRegressor())])	**5.76**	[70.98, 59.4, 54.11, 61.16, 21.1, 53.88, 52.06, 23.64]

Results - Detailed



Method: Univariate Time Series **Flatten to percentile (best results with p75)**	**4CV avgRMSE**	**Predictions on test**
Pipeline(Rocket(random_state=42)), StandardScaler()), RidgeCV()))	5.13	[73.4 62.48 51.78 64.54 24.5 47.43 47.18 25.59]
Pipeline(Rocket(random_state=42)), StandardScaler()), SelectFromModel(estimator=RidgeCV())), RidgeCV()	4.99	[74.22 62.62 51.48 64.58 25.38 47.39 46.56 25.52]
Best model: ROCKET + Noise cleaning + ExtraTreesRegressor Pipeline(Rocket(random_state=42)), StandardScaler()), SelectFromModel(estimator=RidgeCV())), ExtraTreesRegressor())	**4.71**	[72, 59.4, 51.56, 60.18, 22.51, 49.96, 48.72, 22.9]

Results - Best Model



Best model: Samples flattened to p75 (time series with 3424 length)

```
make_pipeline(Rocket(normalise=True, num_kernels=10000, random_state=142),
              StandardScaler(),
              SelectFromModel(RidgeCV()),
              ExtraTreesRegressor(n_estimators=100, random_state=142))
```

CV RMSE: 4.44, CV R2: 0.94
Predictions on test set: **[71.86, 59.64, 53.14, 60.24, 22.78, 51.52, 49.24, 23.8]**
Time to train + test (sec): 20.40 seconds

ROCKET creates 20k features in a tabular feature vector, feature selection with **SelectFromModel(RidgeCV)** reduces them to 7k and ExtraTreesRegressor reduces them to 922 (all other features have 0 feature importance)

Results - Best Model

1. **Outlier removal:** Flatten the time series to p75.	1. **Flatten to percentile**
2. TS transformation: Rocket time series transform to extract features from p75 time series (convolution may have smoothing effects)	**2. ROCKET()**
3. Noise reduction: Scaling and feature selection	**3. StandardScaler()** **SelectFromModel(RidgeCV())**
4. **Learning algorithm:** A non-linear regressor ensemble of randomised decision trees inspired by Random Forests.	**4. ExtraTreesRegressor()**

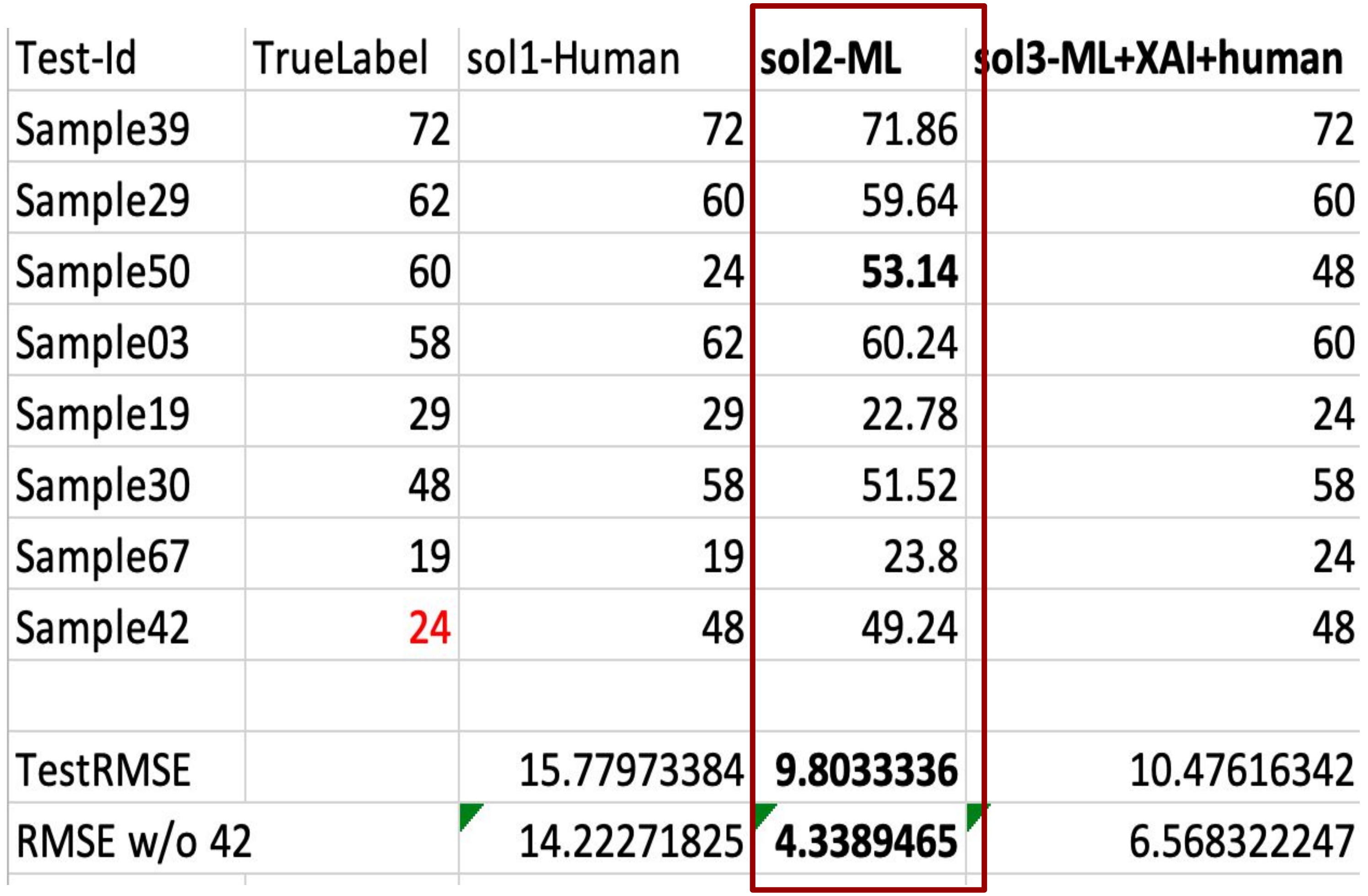
Results - Our Submissions

Our predictions (in the order presented in the test set):

1. Human guess: sol1
2. Best model: sol2
3. Best model + XAI + human: sol3

(presented in PART2)

Our best model avgCV: 4.44
Test error without outlier: 4.33



Test-Id	TrueLabel	sol1-Human	**sol2-ML**	**sol3-ML+XAI+human**
Sample39	72	72	71.86	72
Sample29	62	60	59.64	60
Sample50	60	24	**53.14**	48
Sample03	58	62	60.24	60
Sample19	29	29	22.78	24
Sample30	48	58	51.52	58
Sample67	19	19	23.8	24
Sample42	24	48	49.24	48
TestRMSE		15.77973384	**9.8033336**	10.47616342
RMSE w/o 42		14.22271825	**4.3389465**	6.568322247

Thank you for listening! Questions?

PART 2 - XAI to Improve the Best Predictive Model (presented by Thach)