Karlsruhe Institute of Technology

HELMHOLTZ AI
ARTIFICIAL INTELLIGENCE
COOPERATION UNIT

Non-Sequential Machine Learning Pipelines with pyWATTS

deRSE23 - Conference for Research Software Engineering in Germany

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Machine Learning Pipelines

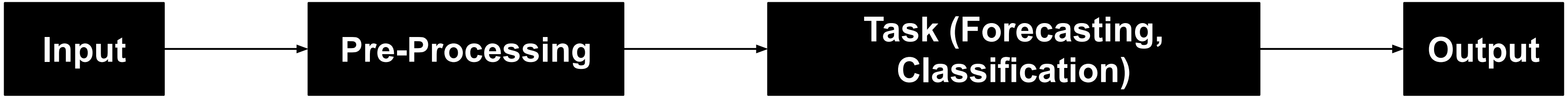
Input

Pre-Processing

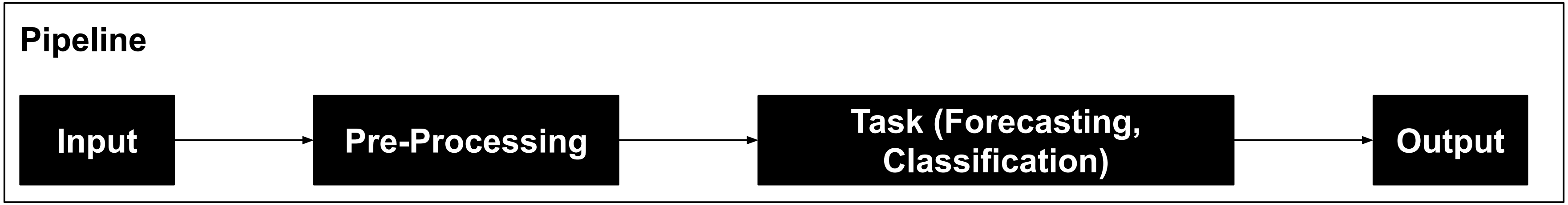
Task (Forecasting, Classification)

Output

Machine Learning Pipelines



Machine Learning Pipelines



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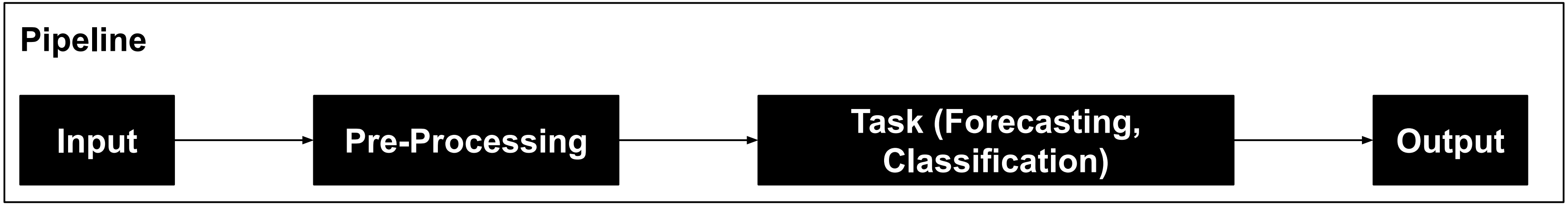

- Why is this beneficial?
  - Hyperparameter tuning is simpler - you can tune the whole pipeline.
  - It is easy to handle - there is only one pipeline object that needs to be saved.
  - You only have to call the *fit* method once to train the entire pipeline.

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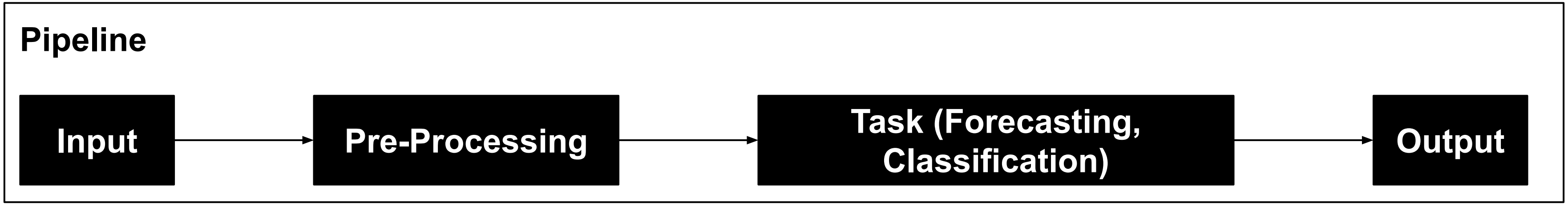

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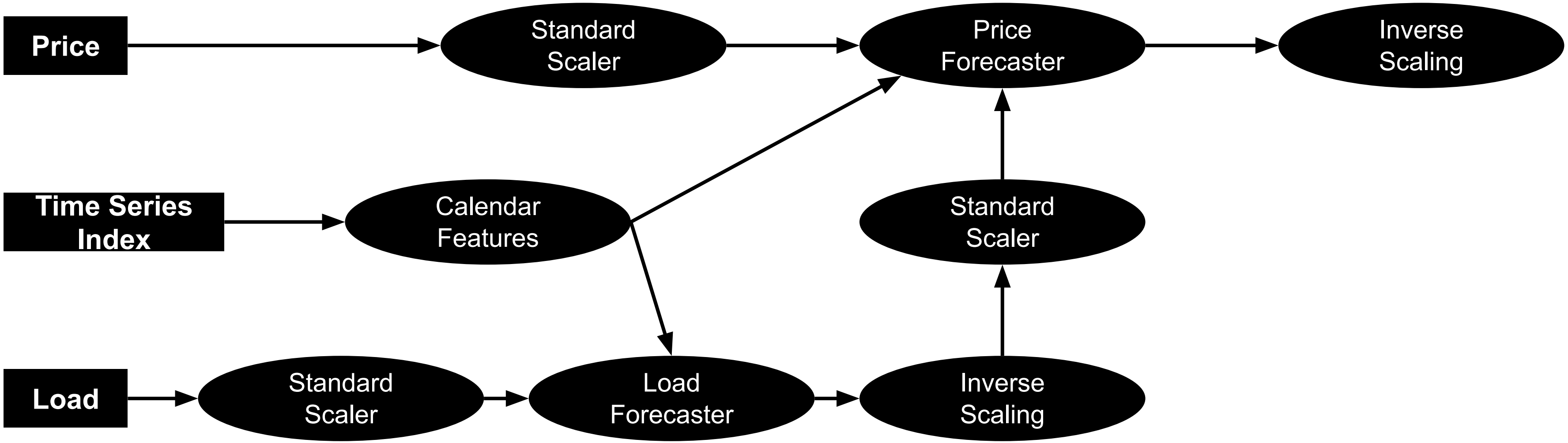
  - You only have to call the *fit* method once to train the entire pipeline.
- Existing sequential pipeline implementations in…
  - sklearn
  - sktime

However: Many use cases are non-sequential

For example, electricity price forecasting



pyWATTS: Python Workflow Automation Tool for Time Series

- pyWATTS models pipeline as directed acyclic graphs enabling non-sequential workflows:
  - Code is easier to write and intuitive to understand.
  - Hyperparameter optimisation is easier.
  - Possible to combine multiple tasks in one pipeline.

- pyWATTS provides three different APIs for creating pipelines:
  - Functional API
  - Imperative API
  - Constructor API

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For Today: Focus on the Functional API

Example of pyWATTS Code

```
pipeline = Pipeline( path="../results" )

calendar = CalendarExtraction( continent="Europe",
                               country="Germany",
                               features=[CalendarFeature.month,CalendarFeature.weekday,
                                         CalendarFeature.weekend],
                               name="calendar"
                               )(x=pipeline[ "load_power_statistics" ])

[... # Extract Lag Features]

forecast_load = SKLearnWrapper( module=LinearRegression( fit_intercept=True), name="load_forecast" )(
    features=lag_features_load,  calendar=calendar,  target=target)

forecast_price_scaled = SKLearnWrapper( module=LinearRegression( fit_intercept=True),
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[... # Evaluate Forecast]

pipeline.train(data)
pipeline.test(data)
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Example of pyWATTS Code

Full example in Jupyter Notebook

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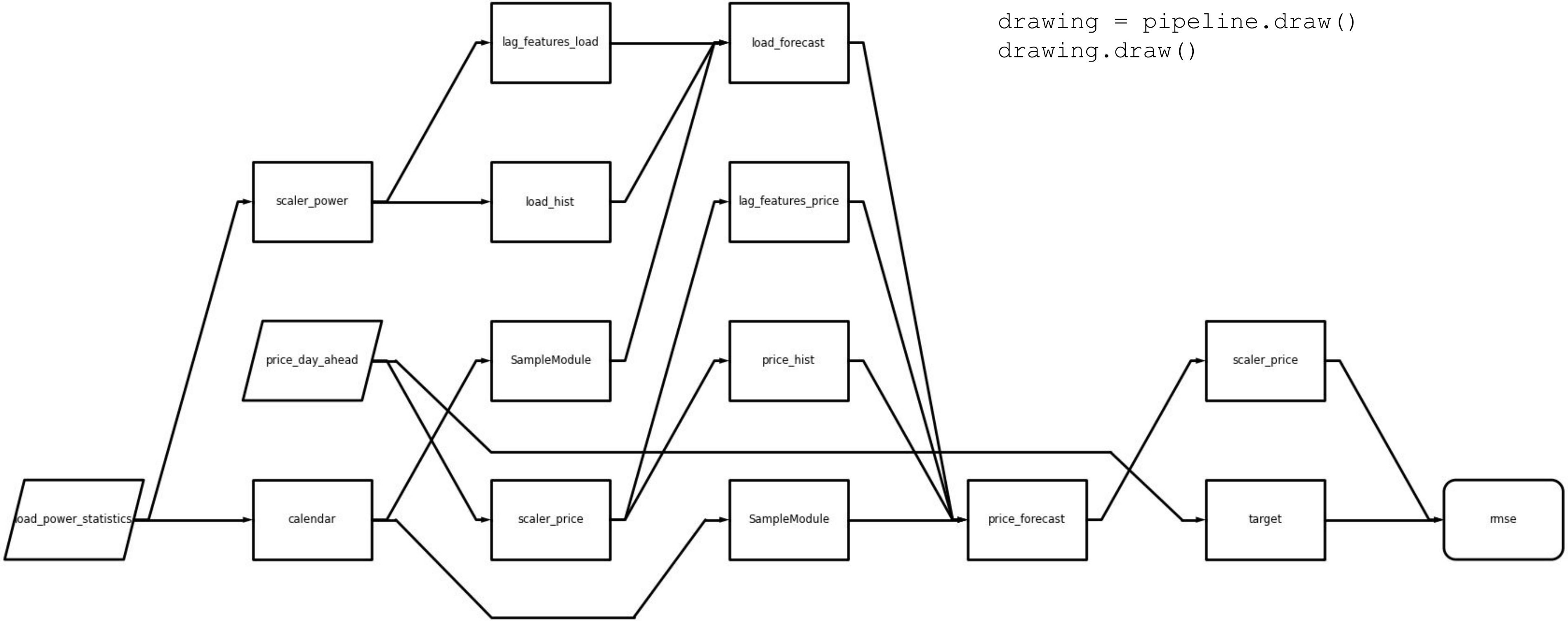
Visualisation of resulting pyWATTS Pipeline




```
drawing = pipeline.draw()
drawing.draw()
```

Easy Hyperparameter Tuning

```
params = {"load forecast  module" : [LinearRegression(), MLPRegressor()],
          "price_forecast__module" : [LinearRegression(), MLPRegressor()],
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from sklearn.model_selection import TimeSeriesSplit
tscv = TimeSeriesSplit( test_size=168*4)
pipeline_cv = GridSearchCV(pipeline, param_grid=params, cv=tscv)
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Out[14]: {'calendar__features': [<CalendarFeature.month_cos: 4>,
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Full example in Jupyter Notebook

Use-Cases Realised With pyWATTS

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- Enhancing anomaly detection methods (**see our poster for more information):**
  - We use latent space data representations of energy time series to improve the performance of anomaly detection methods.
  - Read our anomaly detection paper here!
- (Probabilistic) Profile Neural Network: (Prob)PNN (**see our poster for more information):**
  - We incorporate statistical information in the form of profiles into deep learning methods to improve (probabilistic) time series forecasting.
  - Read the paper on the deterministic PNN here and the probabilistic PNN here!
- AutoPV: Automated Photovoltaic Forecasts:
  - We use information about PV configurations to create a cold-start capable ensemble of PV power forecasting models.
  - Read our AutoPV paper here!
- Creating Probabilistic Forecasts from arbitrary deterministic forecasts:
  - We use a conditional invertible neural network to transform an arbitrary deterministic forecast into a probabilistic forecast.
  - Read our paper on creating probabilistic forecasts here!

Development Roadmap & How to Contribute

Karlsruhe Institute of Technology

- We aim to grow and develop pyWATTS in the coming months by:
  - Integrating further with sktime
  - Increasing performance by enabling parallel execution of pipeline components.

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- We aim to grow and develop pyWATTS in the coming months by:
  - Integrating further with sktime
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- We are looking to grow the pyWATTS community - so if you are interested in contributing please get in touch!
  - Join the pyWATTS community as a user or developer:
    - GitHub - pyWATTS: Python Workflow Automation Tool for Time-Series
    - GitHub - pywatts-pipeline
  - Contact us if you want more information:
    - pywatts-team@iai.kit.edu

Thank you for your Attention

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pyWATTS-pipeline

https://github.com/KIT-IAI/pywatts-pipeline

deRSE Jupyter Notebooks

https://github.com/KIT-IAI/pyWATTS-deRSE-2023

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