Artificial Intelligence in Industry

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Alma Mater Studiorum · University of Bologna

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1 Preliminaries

Problem formalization Defines the ideal goal.

Problem formalization

Solution formalization Defines the actual possible approaches to solve a problem.

Solution formalization

Occam's razor Principle for which, between two hypotheses, the simpler one is usually correct.

Occam's razor

| **Remark.** This approach has less variance and more bias, making it more robust.

2 Low dimensional anomaly detection: Taxi calls

Anomaly Event that deviates from the usual pattern.

Anomaly

Time series Data with an ordering (e.g., chronological).

Time series

2.1 Data

The dataset is a time series and it is a `DataFrame` with the following fields:

`timestamp` with a 30 minutes granularity.

`value` number of calls.

The label is a `Series` containing the timestamps of the anomalies.
An additional `DataFrame` contains information about the time window in which the anomalies happen:

`begin` acceptable moment from which an anomaly can be detected.

`end` acceptable moment from which there are no anomalies anymore.

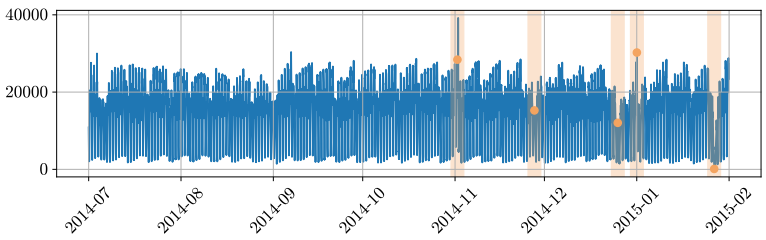


Figure 2.1: Plot of the time series, anomalies, and windows

2.2 Approaches

2.2.1 Gaussian assumption

Assuming that the data follows a Gaussian distribution, mean and variance can be used to determine anomalies through a threshold. z-score can also be used.

2.2.2 Characterize data distribution

Classify a data point as an anomaly if it is too unlikely.

Problem formalization Given a random variable X with values x to represent the number of taxi calls, we want to find its probability density function (PDF) $f(x)$.

An anomaly is determined whether:

$$f(x) \leq \varepsilon$$

where ε is a threshold.

Remark. A PDF can be reasonably used even though the dataset is discrete if its data points are sufficiently fine-grained.

Remark. It is handy to use negated log probabilities as:

- The logarithm adds numerical stability.
- The negation makes the probability an alarm signal, which is a more common measure.

Therefore, the detection condition becomes:

$$-\log f(x) \geq \varepsilon$$

Solution formalization The problem can be tackled using a density estimation technique.

2.2.2.1 Univariate kernel density estimation

Kernel density estimation (KDE)

Kernel density estimation (KDE) Based on the assumption that whether there is a data point, there are more around it. Therefore, each data point is the center of a density kernel.

Density kernel A kernel $K(x, h)$ is defined by:

- The input variable x.
- The bandwidth h.

Gaussian kernel Kernel defined as:

$$K(x, h) \propto e^{-\frac{x^2}{2h^2}}$$

where:

- The mean is 0.
- h is the standard deviation.

As the mean is 0, an affine transformation can be used to center the kernel on a data point μ as $K(x - \mu, h)$.

Given m training data points $\bar{x}_i$, the density of any point x can be computed as the kernel average:

$$f(x, \bar{x}, h) = \frac{1}{m} \sum_{i=0}^{m} K(x - \bar{x}_i, h)$$

Therefore, the train data themselves are used as the parameters of the model while the bandwidth h has to be estimated.

Data split Time series are usually split chronologically:

Train Should ideally contain only data representing the normal pattern. A small amount of anomalies might be tolerated as they have low probabilities.

Validation Used to find the threshold ε.

Test Used to evaluate the model.

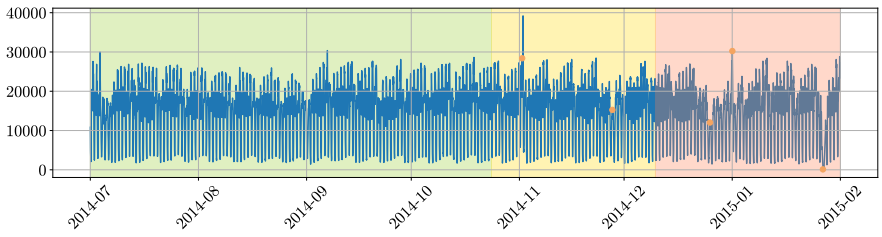


Figure 2.2: Train, validation, and test splits

Metrics It is not straightforward to define a metric for anomaly detection. A cost model to measure the benefits of a prediction is more suited. A simple cost model can be based on:

True positives (`TP`) Windows for which at least an anomaly is detected;

False positives (`FP`) Detections that are not actually anomalies;

False negatives (`FN`) Undetected anomalies;

Advance (`adv`) Time between an anomaly and when it is first detected;

and is computed as:

$$(c_{\text{false}} \cdot \texttt{FP}) + (c_{\text{miss}} \cdot \texttt{FN}) + (c_{\text{late}} \cdot \texttt{adv}_{\leq 0})$$

where c_{false}, c_{miss}, and c_{late} are hyperparameters.

Bandwidth estimation According to some statistical arguments, a rule-of-thumb to estimate h in the univariate case is the following:

$$h = 0.9 \cdot \min\left\{\hat{\sigma}, \frac{\texttt{IQR}}{1.34}\right\} \cdot m^{-\frac{1}{5}}$$

where:

- `IQR` is the inter-quartile range.
- $\hat{\sigma}$ is the standard deviation computed over the whole dataset.

Threshold optimization Using the train and validation set, it is possible to find the best threshold ε that minimizes the cost model through linear search.

> **Remark.** The train set can be used alongside the validation set to estimate ε as this operation is not used to prevent overfitting.

> **Remark.** The evaluation data should be representative of the real world distribution. Therefore, in this case, to evaluate the model the whole dataset can be used.

> **Remark.** KDE assumes that the Markov property holds. Therefore, each data point is considered independent to the others.

2.2.2.2 Multivariate kernel density estimation

Remark. In this dataset, nearby points tend to have similar values.

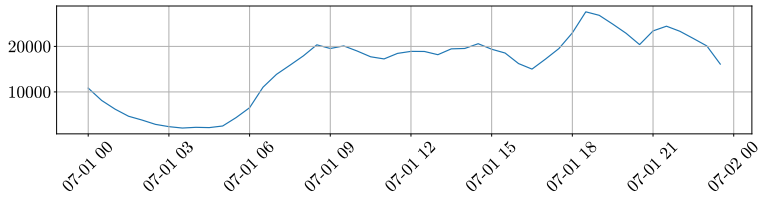


Figure 2.3: Subset of the dataset

Autocorrelation plot Plot to visualize the correlation between nearby points of a series. Given the original series, it is duplicated, shifted by a lag l, and the Pearson correlation coefficient is then computed between the two series. This operation is repeated over different values of l.

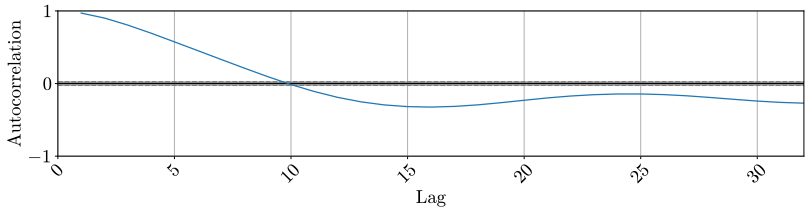


Figure 2.4: Autocorrelation plot of the subset of the dataset. There is strong correlation up to 4-5 lags.

Sliding window Given a window size w and a stride s, the dataset is split into sequences of w continuous elements.

Remark. Incomplete sequences at the start and end of the dataset are ignored.

Remark. In `pandas`, the `rolling` method of `Dataframe` allows to create a slicing window iterator. This approach creates the windows row-wise and also considers incomplete windows. However, a usually more efficient approach is to construct the sequences column-wise by hand.

Multivariate KDE Extension of KDE to vector variables.

Window size estimation By analyzing the autocorrelation plot, an ideal window size can be picked as the lag with a low correlation (e.g., 10 according to Figure 2.4).

Bandwidth estimation Differently from the univariate case, the bandwidth has to be estimated by maximizing the log-likelihood on the validation set. Given:

- The validation set $\tilde{x}$,
- The observations x,
- The bandwidth h,
- The density estimator $\hat{f}$

the likelihood is computed, by assuming independent observations, as:

$$L(h, x, \tilde{x}) = \prod_{i=1}^{m} \hat{f}(x_i, \tilde{x}_i, h)$$

Maximum likelihood estimation is defined as:

$$\arg\max \mathbb{E}_{x\sim f(x),\tilde{x}\sim f(x)}[L(h,x,\tilde{x})]$$

where $f(x)$ is the true distribution.

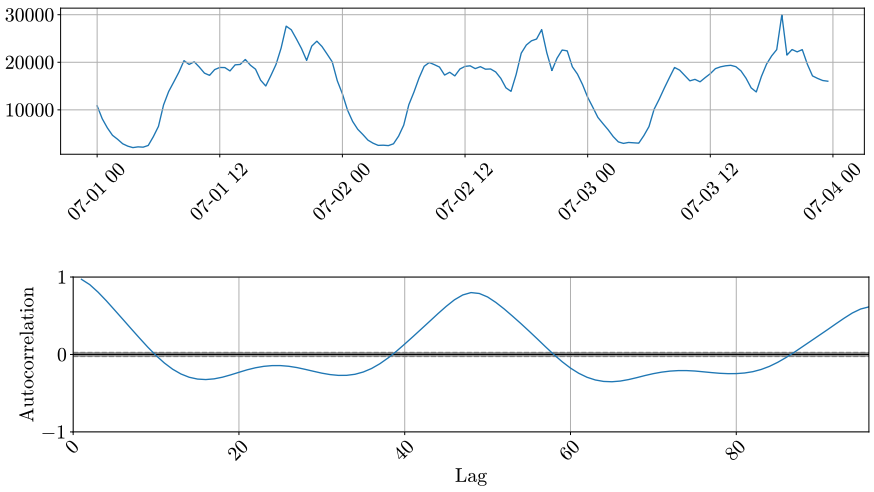
In practice, the expected value is sampled from multiple validation and training sets through cross-validation and grid-search.

Remark. As different folds for cross-validation must be tried, grid-search is an expensive operation.

Threshold optimization The threshold can be determined as in Section 2.2.2.1.

2.2.2.3 Time-dependent estimator

The approach taken in Sections 2.2.2.1 and 2.2.2.2 is based on the complete timestamp of the dataset. Therefore, the same times on different days are treated differently. However, it can be seen that this time series is approximately periodic, making the approach used so far more complicated than necessary.



Time input It is possible to take time into consideration by adding it as a parameter of the density function:

$$f(t,x)$$

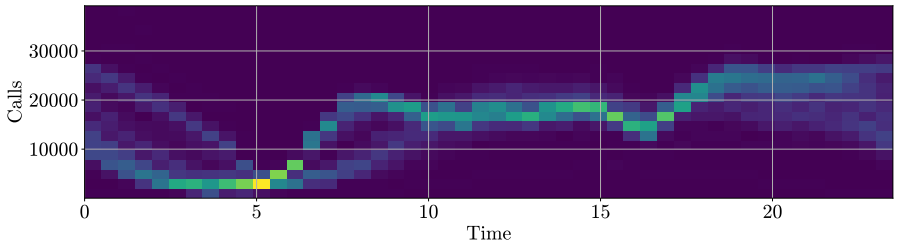


Figure 2.5: 2D histogram of the distribution. Lighter colors indicate a higher frequency of occurrence.

However, t is a controlled variable and is completely predictable (i.e., if times are samples with different frequencies, they should not affect the overall likelihood). Therefore, a conditional density should be used:

$$f(x \mid t) = \frac{f(t, x)}{f(t)}$$

where $f(t)$ can be easily computed using KDE on the time data.

> **Remark.** For this dataset, the time distribution is uniform. Therefore, $f(t)$ is a constant and it is correct to use $f(t, x)$ as the estimator.

Bandwidth estimation The bandwidth can be estimated as in Section 2.2.2.2.

> **Remark.** When using the `scikit-learn`, the dataset should be normalized as the implementation of KDE use the same bandwidth for all features.

Threshold optimization The threshold can be determined as in Section 2.2.2.1.

2.2.2.4 Time-indexed model

Ensemble model Model defined as: Ensemble model

$$f_{g(t)}(x)$$

where:

- f_i are estimators, each working on subsets of the dataset and solving a smaller problem.
- $g(t)$ determines which particular f_i should solve the input.

Time-indexed model Consider both time and sequence inputs by using an ensemble model. Each estimator is specialized on a single time value (i.e., an estimator for `00:00`, one for `00:30`, ...).

Bandwidth estimation The bandwidth can be estimated as in Section 2.2.2.2.

Threshold optimization The threshold can be determined as in Section 2.2.2.1.

3 High dimensional anomaly detection: HPC centers

3.1 Data

The dataset is a time series with the following fields:

`timestamp` with a 5 minutes granularity.

HPC data technical data related to the cluster.

`anomaly` indicates if there is an anomaly.

In practice, the cluster has three operational modes:

Normal the frequency is proportional to the workload.

Power-saving the frequency is always at the minimum.

Performance the frequency is always at the maximum.

For this dataset, both power-saving and performance are considered anomalies.

3.1.1 High-dimensional data visualization

Individual plots Plot individual columns.

Statistics Show overall statistics (e.g., `pandas describe` method)

Heatmap Heatmap with standardized data.

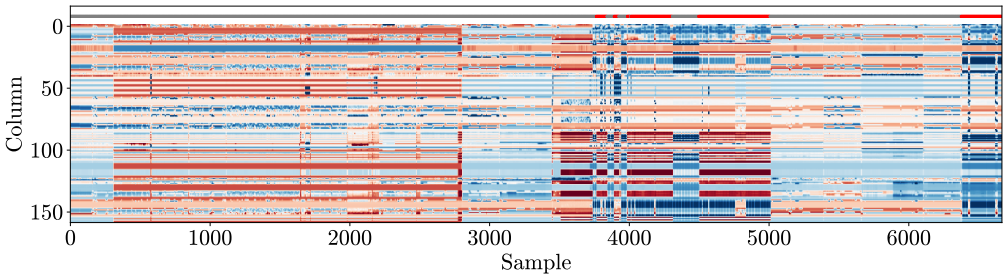


Figure 3.1: Heatmap of the dataset. On the top line, gray points represent normal behavior while red points are anomalies. In the heatmap, white tiles represent the mean, red tiles represent values below average, and blue tiles represent values above average.

3.2 Approaches

3.2.1 Multivariate KDE

Given the train, validation, and test splits, the dataset is standardized using the training set alone. This avoids leaks from the test set.
The KDE model, bandwidth, and threshold are fitted as in Chapter 2.

Cost model A simple cost model can be based on:

- False positives,
- False negatives,
- A time tolerance.

Problems KDE on this dataset has the following problems:

- It is highly subject to the curse of dimensionality and requires more data to be reliable.

  Remark. KDE does not compress the input features and grows with the training set. In other words, it has low bias and high variance.

- As the dataset is used during inference, a large dataset is computationally expensive (with time complexity $O(mn)$, where m is the number of dimensions and n the number of samples).
- It only provides an alarm signal and not an explanation of the anomaly. In low-dimensionality, this is still acceptable, but with high-dimensional data it is harder to find an explanation.

3.2.2 Gaussian mixture model

Gaussian mixture model (GMM)

Gaussian mixture model (GMM) Selection-based ensemble that estimates a distribution as a weighted sum of Gaussians. It is assumed that data can be generated by the following probabilistic model:

$$X_Z$$

where:

- X_k are random variables following a multivariate Gaussian distribution. The number of components is a hyperparameter that can be tuned to balance bias-variance.
- Z is a random variable representing the index k of the variable X to use to generate data.

More specifically, the PDF of a GMM g is defined as:

$$g(x, \mu, \Sigma, \tau) = \sum_{k=1}^{n} \tau_k f(x, \mu_k, \Sigma_k)$$

where:

- f is the PDF of a multivariate normal distribution.
- μ_k and Σ_k are the mean and covariance matrix for the k-th component, respectively.
- τ_k is the weight for the k-th component and corresponds to $\mathcal{P}(Z = k)$.

Training Likelihood maximization can be used to train a GMM to approximate another distribution:

$$\arg\max_{\mu,\Sigma,\tau} \mathbb{E}_{x\sim X}\left[L(x,\mu,\Sigma,\tau)\right] \qquad \text{subject to } \sum_{k=1}^{n}\tau_k = 1$$

where the expectation can be approximated using the training set (i.e., empirical risk minimization):

$$\mathbb{E}_{x\sim X}\left[L(x,\mu,\Sigma,\tau)\right] \approx \prod_{i=1}^{m} g(x_i,\mu,\Sigma,\tau)$$

Remark. Empirical risk minimization can be solved in two ways:

- Use a single large sample (traditional approach).
- Use many smaller samples (as in cross-validation).

By putting the definitions together, we obtain the following problem:

$$\arg\max_{\mu,\Sigma,\tau} \prod_{i=1}^{m}\sum_{k=1}^{n}\tau_k f(x,\mu_k,\Sigma_k) \qquad \text{subject to } \sum_{k=1}^{n}\tau_k = 1$$

which:

- Cannot be solved using gradient descent as it is an unconstrained method.
- Cannot be solved using mixed-integer linear programming as the problem is non-linear.
- Cannot be decomposed as the variables μ, Σ, and τ appear in every term.

It is possible to simplify the formulation of the problem by introducing new variables:

- A new latent random variable Z_i is added for each example. $Z_i = k$ iff the i-th example is drawn from the k-th component. The PDF of the GMM can be reformulated to use Z_i and without the summation as:

  $$\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau) = \tau_{z_i} f(x,\mu_k,\Sigma_k)$$

  The expectation becomes:

  $$\mathbb{E}_{x\sim X,\{z_i\}\sim\{Z_i\}}\left[L(x,z,\mu,\Sigma,\tau)\right] \approx \mathbb{E}_{\{z_i\}\sim\{Z_i\}}\left[\prod_{i=1}^{m}\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau)\right]$$

  Note that, as the distributions to sample z_i are unknown, Z_i cannot be approximated in the same way as X.

- New variables $\tilde{\tau}_{i,k}$ are introduced to represent the distribution of the Z_i variables. In other words, $\tilde{\tau}_{i,k}$ corresponds to $\mathcal{P}\left(Z_i = k\right)$. This allows to approximate the expectation as:

  $$\mathbb{E}_{\hat{x}\sim X,\hat{z}\sim Z}\left[L(\hat{x},\hat{z},\mu,\Sigma,\tau)\right] \approx \prod_{i=1}^{m}\prod_{k=1}^{n}\tilde{g}_i(x_i,z_i,\mu,\Sigma,\tau)^{\tilde{\tau}_{i,k}}$$

  The intuitive idea is that, if Z_i is sampled, $\tilde{\tau}_{i,k}$ of the samples would be the k-th component. Therefore, the corresponding density should be multiplied by itself for $\tilde{\tau}_{i,k}$ times.

Finally, the GMM training can be formulated as follows:

$$\arg\max_{\mu,\Sigma,\tau,\tilde{\tau}} \prod_{i=1}^{m}\prod_{k=1}^{n} \tilde{g}_i(x_i, z_i, \mu, \Sigma, \tau)^{\tilde{\tau}_{i,k}} \quad \text{s.t.} \quad \sum_{k=1}^{n} \tau_k = 1, \forall i = 1 \dots m : \sum_{k=1}^{n} \tilde{\tau}_{i,k} = 1$$

which can be simplified by applying a logarithm and solved using expectation-maximization.

Remark. Differently from KDE, GMM allows making various types of prediction:

- Evaluate the (log) density of a sample.
- Generate a sample.
- Estimate the probability that a sample belongs to a component.
- Assign samples to a component (i.e., clustering).

Remark. GMM can be seen as a generalization of k-means.

Remark. Differently from KDE, most of the computation is done at training time.

Number of components estimation The number of Gaussians to use in GMM can be determined through grid-search and cross-validation.

Remark. Other method such as the elbow method can also be applied. Some variants of GMM are able to infer the number of components.

Threshold optimization The threshold can be determined in the same way as in Section 2.2.2.1.

3.2.3 Autoencoder

Autoencoder Neural network trained to reconstruct its input. It is composed of two components: Autoencoder

Encoder $e(x, \theta_e)$ that maps an input x into a latent vector z.

Decoder $d(z, \theta_d)$ that maps z into a reconstruction of x.

Training Training aims to minimize the reconstruction MSE:

$$\arg\min_{\theta_e,\theta_d} \|d\left(e(x_i, \theta_e), \theta_d\right) - x_i\|_2^2$$

To avoid trivial embeddings, the following can be done:

- Use a small-dimensional latent space.
- Use L1 regularization to prefer sparse encodings.

Autoencoder for anomaly detection By evaluating the quality of the reconstruction, an autoencoder can be used for anomaly detection:

$$\|x - d(e(x, \theta_e), \theta_d)\|_2^2 \geq \varepsilon$$

The advantages of this approach are the following:

- The size of the neural network does not scale with the training data.
- Neural networks have good performances in high-dimensional spaces.
- Inference is fast.

However, the task of reconstruction can be harder that density estimation.

Remark. It is always a good idea to normalize the input of a neural network to have a more stable gradient descent. Moreover, with normalized data, common weight initialization techniques make the output approximately normalized too.

Remark. Counterintuitively, neural networks have a higher bias compared to traditional machine learning techniques for mainly two reasons:

- A change in a single parameter affects the whole network.
- Training using SGD inherently prevents overfitting.

Theorem 3.2.1. Under the following assumptions:

- Normally distributed noise (i.e., distance between prediction and ground truth),
- Independent noise among each output component (i.e., columns),
- Same variance (i.e., homoscedasticity) in the noise of each output component,

autoencoders are trained as density estimators.

Remark. When minimizing MSE, these assumptions hold.

Proof. When training an autoencoder h using MSE on m examples with n features, the following problem is solved:

$$\begin{aligned}
\arg\min_\theta \|h(\mathbf{x},\theta)-\mathbf{x}\|_2^2 &= \arg\min_\theta \sum_{i=1}^{m}\sum_{j=1}^{n}(h_j(\mathbf{x}_i,\theta)-\mathbf{x}_{i,j})^2 \\
&= \arg\min_\theta \log\exp\left(\sum_{i=1}^{m}\sum_{j=1}^{n}(h_j(\mathbf{x}_i,\theta)-\mathbf{x}_{i,j})^2\right) \\
&= \arg\min_\theta \log\prod_{i=1}^{m}\exp\left(\sum_{j=1}^{n}(h_j(\mathbf{x}_i,\theta)-\mathbf{x}_{i,j})^2\right) \\
&= \arg\min_\theta \log\prod_{i=1}^{m}\exp\left((h(\mathbf{x}_i,\theta)-\mathbf{x}_i)^T\boldsymbol{I}(h(\mathbf{x}_i,\theta)-\mathbf{x}_i)\right)
\end{aligned}$$

The following adjustments can be done without altering the problem:

- Negate the argument of exp and solve a maximization problem,
- Multiply the argument of exp by $\frac{1}{2}\sigma$, for some constant σ,
- Multiply exp by $\frac{1}{\sqrt{2\pi\sigma}}$.

The problem becomes:

$$\arg\max_\theta \log\prod_{i=1}^{m}\frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{1}{2}(h(\mathbf{x}_i,\theta)-\mathbf{x}_i)^T(\sigma\boldsymbol{I})(h(\mathbf{x}_i,\theta)-\mathbf{x}_i)\right)$$

which is the PDF of a multivariate normal distribution $f(\mathbf{x}_i, h(\mathbf{x}_i), \sigma\boldsymbol{I})$ with a diagonal covariance matrix. More specifically, this is a distribution:

- Centered on $h(\mathbf{x}_i)$,
- With independent normal components,

- With components with uniform variance.

Therefore, when using MSE as loss, training is a likelihood maximization problem. □

Threshold optimization The threshold can be determined in the same way as in Section 2.2.2.1.

Multiple signal analysis With autoencoders, it is possible to compare the reconstruction error of single components.

> **Remark.** In most cases, reconstruction errors are often concentrated on a few features.

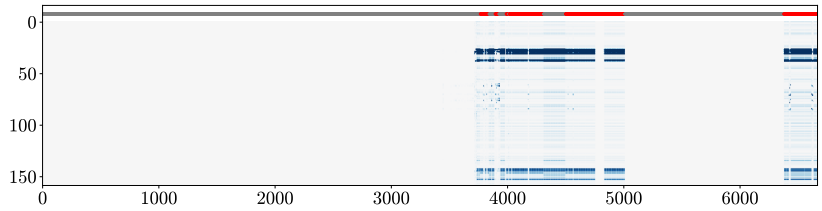


Figure 3.2: Reconstruction error of each feature

> **Remark.** It is possible to rank the feature with the highest reconstruction error to provide more insights.

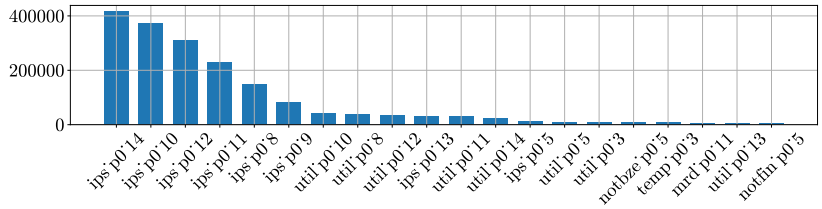


Figure 3.3: Top-20 features with the largest error

> **Remark.** In industrial use-cases, a usually well working approach consists of building an estimator for the sensors. More specifically, observed variables can be split into:
>
> - Controlled variables x_c.
> - Measured variables x_s.
>
> During anomaly detection, controlled variables should not be used to determine anomalous behaviors. In addition, there is a causal relation between the two groups as measured variables are caused by the controlled variables ($x_c \to x_s$).
> A well working method is to use a regressor f as a causal model, such that:
>
> $$x_s \approx f(x_c; \theta)$$

4 Missing data: Traffic data

4.1 Data

Time series on traffic anomalies with missing values.

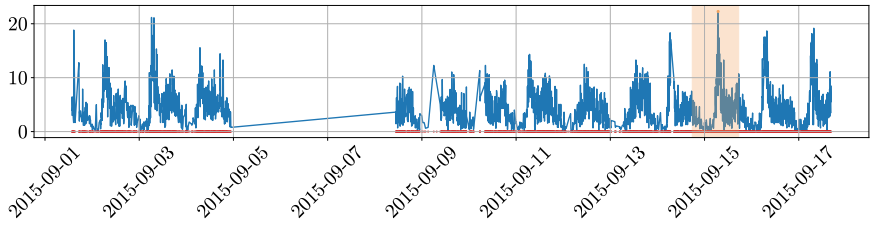


Figure 4.1: Plot of the data. Straight lines are artifacts of missing values. Red dots below represent the actual data points.

4.2 Preliminaries

The dataset has sparse indexes (i.e., indexes are non-contiguous) and missing values are represented by gaps. It is necessary to use dense indexes where missing values are explicitly marked as `NaN`.

4.2.1 Resampling / Binning

Resampling / binning Resample the indexes of the dataset so that they have a regular step (e.g., 5 minutes).

Resampling / binning

| **Remark.** Values that end up in the same bin need to be aggregated (e.g., mean).

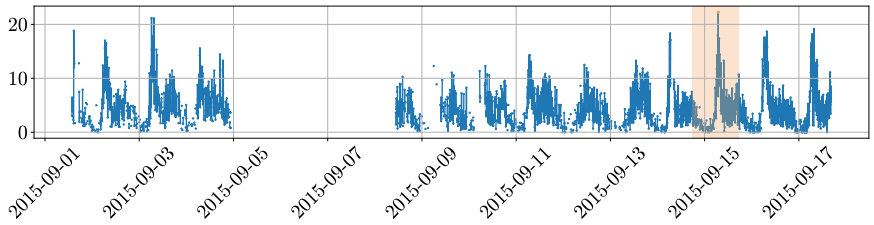


Figure 4.2: Plot of the resampled data without artifacts

4.3 Approaches

Benchmark dataset A portion of known data where some values are artificially removed can be used to evaluate a filling method. As accuracy metric, RMSE can be used.

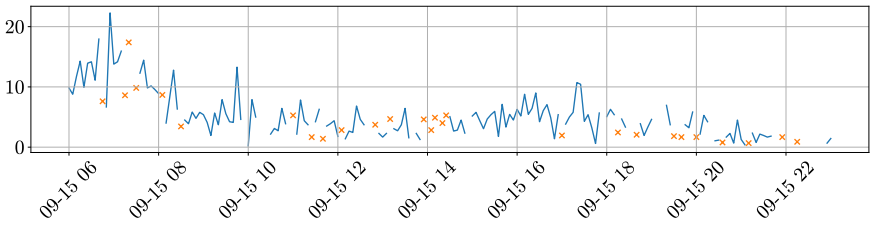


Figure 4.3: Benchmark dataset. Marked points have been artificially removed.

4.3.1 Forward/Backward filling

Forward filling Set the missing value to the last valid observation.

Backward filling Set the missing value to the next valid observation.

Remark. The idea of this approach is that time series usually have strong local correlation (i.e., some sort of inertia).

Remark. Forward/backward filling tend to work well on low variance portions of the data.

4.3.2 Geometric interpolation

Interpolate a function to determine missing points. Possible methods are:

- Linear,
- Nearest value,
- Polynomial,
- Spline.

Remark. (R)MSE assumes that the data is normally distributed, independent, and with the same variability at all points. This is not usually true with time series.

4.3.3 Density estimator

A density estimator can be used to determine a distribution from all the available data. Given an estimator $f(x, \theta)$ for $\mathcal{P}(x)$, predictions can be obtained through maximum a posteriori (MAP):

$$\arg\max_x f(x, \theta)$$

However, MAP with density estimators is computationally expensive.

Remark. Almost all inference approaches in machine learning can be reduced to a maximum a posteriori computation.

4.3.4 Regressor

A regressor can be used to fill missing values autoregressively through a rolling forecast by repeatedly making a prediction and including the new point as a training sample. However, regression only relies on the data on one side (past or future) and each autoregressive iteration accumulates compound errors.

4.3.5 Gaussian processes

Remark. The ideal estimator is the one that is:

- At least as powerful as interpolation (i.e., considers both past and future data).
- Able to detect the expected variability (i.e., a measure of confidence).

Gaussian process

Gaussian process Stochastic process (i.e., collection of indexed random variables) such that:

- The index variables x are continuous and represents an input of arbitrary dimensionality.
- The variable y_x represents the output for x.

The random variables y_x respect the following assumptions:

- They follow a Gaussian distribution.
- The standard deviation depends on the distance between a point and the given observations (i.e., a confidence measure).
- y_xs are correlated. Therefore, every finite subset of y_x variables follows a multivariate normal distribution.

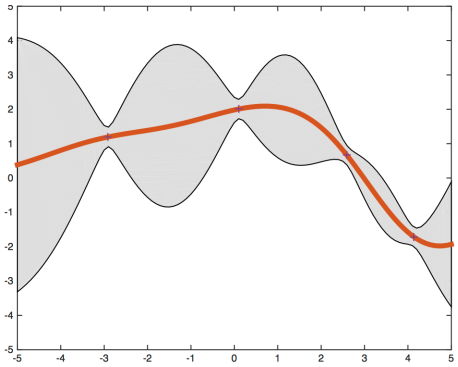


Figure 4.4: Example of Gaussian process. The red line represents the mean and the gray area the confidence interval.

Remark. The PDF of a multivariate normal distribution is defined by the mean vector $\boldsymbol{\mu}$ and the covariance matrix $\boldsymbol{\Sigma}$. By recentering ($\boldsymbol{\mu} = \bar{\mathbf{0}}$), knowing $\boldsymbol{\Sigma}$ is enough to compute the joint or conditional density.

Remark. To fill missing values, the conditional density $f(y_x|\bar{y}_{\bar{x}})$ is used to infer a new observation y_x given a set of known observations $\bar{y}_x$.

Naive implementation

Training Given the training observations $\bar{y}_x$, the covariance matrix can be defined as a parametrized function $\boldsymbol{\Sigma}(\theta)$ and optimized for maximum likelihood:

$$\arg\max_{\theta} f(\bar{y}_{\bar{x}}, \theta)$$

where f is the joint PDF of a multivariate normal distribution.

Inference To infer the variable y_x associated to an input x, the joint distribution $f(y_x|\bar{y}_{\bar{x}})$ has to be computed:

$$f(y_x|\bar{y}_{\bar{x}}) = \frac{f(y_x, \bar{y}_{\bar{x}})}{f(\bar{y}_{\bar{x}})}$$

- $f(\bar{y}_{\bar{x}})$ can be computed using the $\mathbf{\Sigma}$ determined during training, which is an $n \times n$ matrix assuming n training observations.
- $f(y_x, \bar{y}_{\bar{x}})$ introduces an additional variable and would require an $(n+1) \times (n+1)$ covariance matrix which cannot be determined without further assumptions.

Kernel implementation It is assumed that the covariance of two variables can be determined through parametrized kernel functions $K_\theta(x_i, x_j)$.

> **Remark.** Typically, the kernel is a distance measure.

Training Given the training observations $\bar{y}_x$ and a parametrized kernel function $K_\theta(x_i, x_j)$, training is done by optimizing the kernel for maximum likelihood (e.g., gradient descent).

The trained model is represented by both the kernel parameters θ and the training samples $\bar{y}_x$.

Inference Given a new input x, the joint distribution $f(y_x|\bar{y}_{\bar{x}})$ can be computed by obtaining $\mathbf{\Sigma}_{\bar{x}}$ and $\mathbf{\Sigma}_{x,\bar{x}}$ using the kernel.

Common kernels

Radial basis function Based on the Euclidean distance $d(x_i, x_j)$ between the input points:

$$K(x_i, x_j) = e^{-\frac{d(x_i,x_j)^2}{2l}}$$

where l is a parameter and represents the scale.

White kernel Captures the noise in the data:

$$K(x_i, x_j) = \begin{cases} \sigma^2 & \text{iff } x_i = x_j \\ 0 & \text{otherwise} \end{cases}$$

where σ is a parameter and represents the noise level.

Constant kernel Represents a learnable constant factor, useful to tune the magnitude of other kernels.

Exp-Sine-Squared Captures a period:

$$K(x_i, x_j) = e^{-2\frac{\sin^2\left(\pi\frac{d(x_i,x_j)}{p}\right)}{l^2}}$$

where l and p are parameters representing periodicity and scale, respectively.

Dot product Is more or less able to capture a trend:

$$K(x_i, x_j) = \sigma^2 + x_i x_j$$

where σ is a parameter and represents the base level of correlation.

> **Remark.** This kernel is not translation-invariant

> **Remark.** Bounding the domain of the parameters of a kernel can help control training.

> **Remark.** With Gaussian processes, as we have both the prediction and the confidence interval, likelihood can be used as evaluation metric.

Remark. With Gaussian processes, by predicting points far away from the training observations (i.e., extrapolation), the mean starts to fall to 0. Only when there is a period, predictions outside the reference observations can be reasonably made.

Remark. As the reference observations and the trained kernel are detached, it is possible to change reference observations without retraining.

Inference As changing reference observations can be done without retraining the kernel, the whole series can be used when doing inference to obtain more accurate results.

To fill missing values, there are two main strategies:

Prediction Use the mean as filling value.

Sampling Use mean and variance to sample a point to fill the missing value. Clipping might be needed to make the sampled point valid (e.g., prevent negative values for traffic).

Remark. Using the mean results in a smoother filling, while sampling produces more realistic data.

4.3.6 Multiplicative ensemble

Remark. Gaussian process alone only accounts for covariance and do not consider input-dependent variance (i.e., variance of the traffic at the same week day and time on different days).

Remark. Variance scales via multiplication but not summation:

$$Var(x + \alpha) = Var(x) \qquad Var(\alpha x) = \alpha^2 Var(x)$$

for a constant α.

Multiplicative ensemble Product of the outputs of two models f and g:

$$g(x, \lambda) f(x, \theta)$$

More specifically, the training process aims to obtain:

$$g(x_i, \lambda) f(x_i, \theta) \approx y_i \Rightarrow f(x_i, \theta) \approx \frac{y_i}{g(x_i, \lambda)}$$

In other words, f is trained on a series with variance altered by g.

For this specific problem, f is a Gaussian process and g a standard deviation model.

Standard deviation model A simple standard deviation model consists of mapping time intervals to their standard deviations. This approach is sensitive to the choice of the granularity of the interval (time unit in this problem):

- If it has too many missing values or too little samples, it is not enough to compute a reliable standard deviation.
- If it is too coarse, the computed standard deviation is not useful.

Remark. From empirical considerations, the central limit theorem is observable starting from 30 samples. Therefore, 30 data points are enough to make a reasonably stable prediction of the standard deviation.

As the final model might be too coarse, the following can be done:

Upsampling Use a finer grain unit (i.e., x-axis, time unit in this problem) and fill missing values through linear interpolation.

Smoothing Smooth the upsampled data through a low-pass filter.

For this problem, an exponentially weighted moving average works best as recent data are more relevant.

5 Remaining useful life: Turbofan engines

Maintenance can be of three types:

Reactive maintenance Repair when something is broken.

Preventive maintenance Periodically change something, in a conservative way, before it breaks.

Predictive maintenance Change when something is close to break.

Remaining useful life (RUL) is a metric useful for predictive maintenance.

5.1 Data

The dataset contains run-to-failure experiments on NASA turbofan engines. Excluding domain specific features, the main columns are:

`machine` Index of the experiment.

`cycle` Time step of the experiment.

`rul` Remaining useful life.

From the dataset heatmap, the following can be observed:

- Rows with a uniform blue or red color represent features that contain frequent short-lived variations (i.e., peeks) that skew the standard deviation.
- Some features show a trend synced with the experiments (see rows around 15 at the y-axis with blue peeks at the end of each experiment).

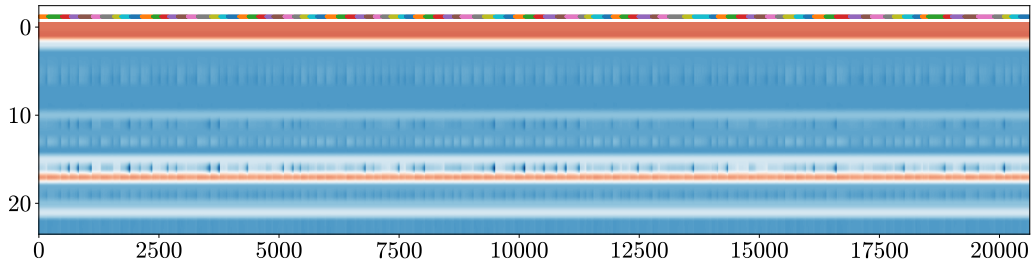


Figure 5.1: Heatmap of the dataset. On the top line, each section represents an experiment.

5.1.1 Data splitting

As the dataset is composed of experiments, standard random sampling will mix experiments and leak information. Therefore, sampling is done on the experiments in chronological order (train first).

Remark. When splitting, the train data should be representative of the test data. Moreover, the test set should be representative of the real world.

5.2 Approaches

5.2.1 Regressor

Predict RUL with a regressor f and set a threshold to trigger maintenance:

$$f(x, \theta) \leq \varepsilon$$

Linear regression A linear regressor can be used as a simple baseline for further experiments.

Remark. For convenience, a neural network without hidden layers can be used as the regressor.

Remark. Training linear models with gradient descent tend to be slower to converge.

Multi-layer perceptron Use a neural network to solve the regression problem.

Remark. A more complex model causes more training instability as it is more prone to overfitting (i.e., more variance).

Remark. Being more expressive, deeper models tend to converge faster.

Remark (Self-similarity curves)**.** Exponential curves (e.g., the loss decrease plot) are self-similar. By considering a portion of the full plot, the subplot will look like the whole original plot.

Remark (Common batch size reason)**.** A batch size of 32 follows the empirical statistical rule of 30 samples. This allows to obtain more stable gradients as irrelevant noise is reduced.

Convolutional neural network Instead of feeding the network a single state, a sequence can be packed as the input using a sliding window as in Section 2.2.2.2. 1D convolutions can then be used to process the input so that time proximity can be exploited.

Remark. Using sequence inputs might expose the model to more noise.

Remark. Even if the dataset is a time series, it is not always the case (as in this problem) that a sequence input is useful.

Remark. The accuracy of the trained regressors are particularly poor at the beginning of the experiments due to the fact that faulty effects are noticeable only after a while. However, we are interested in predicting when a component is reaching its end-of-life. Therefore, wrong predictions when the RUL is high are acceptable.

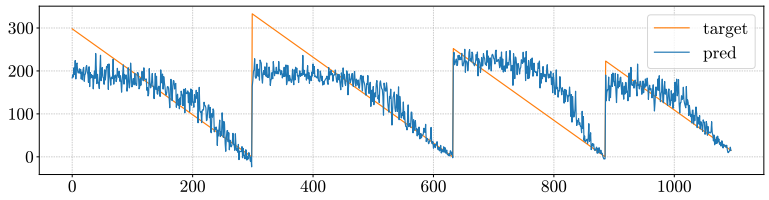


Figure 5.2: Predictions on a portion of the test set

Cost model Intuitively, a cost model can be defined as follows:

- The steps of the experiments are considered as the atomic value units.
- The cost for a failure (i.e., untriggered maintenance) is high.
- Triggering a maintenance too early also has a cost.

Threshold estimation To determine the threshold ε that determines when to trigger a maintenance, a grid-search to minimize the cost model can be performed.

Formally, given a set of training experiments K, the overall problem to solve is the following:

$$\arg\min_{\varepsilon} \sum_{k=1}^{|K|} \texttt{cost}(f(\mathbf{x}_k, \boldsymbol{\theta}^*), \varepsilon)$$
$$\text{subject to } \boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}(f(\mathbf{x}_k, \boldsymbol{\theta}), y_k)$$

Note that ε do not appear in the regression problem. Therefore, this problem can be solved as two sequential subproblems (i.e., regression and then threshold optimization).

5.2.2 Classifier

Predict RUL with a classifier f_ε (for a chosen ε) that determines whether a failure will occur in ε steps:

$$f_\varepsilon(x, \theta) = \begin{cases} 1 & \text{failure in } \varepsilon \text{ steps} \\ 0 & \text{otherwise} \end{cases}$$

Remark. Training a classifier might be easier than a regressor.

Logistic regression A logistic regressor can be uses as baseline.

Remark. For convenience, a neural network without hidden layers can be used as the classifier.

Multi-layer perceptron Use a neural network to solve the classification problem.

Remark. As classifiers output a probability, they can be interpreted as the probability of not failing.

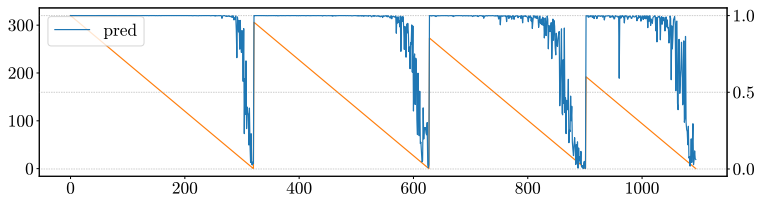
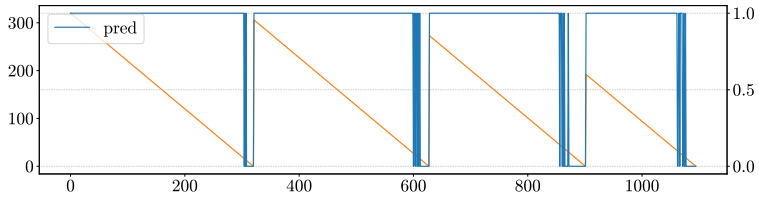


Figure 5.3: Output probabilities of a classifier

By rounding, it is easier to visualize a threshold:



Cost model As defined in Section 5.2.1.

Threshold estimation

Remark. The possibility of using a user-defined threshold ε allows choosing how close to a failure maintenance has to be done. However, early signs of a failure might not be evident at some thresholds so automatically optimizing it might be better.

Formally, given a set of training experiments K, the overall problem to solve is the following:

$$\arg\min_{\varepsilon} \sum_{k=1}^{|K|} \texttt{cost}\left(f(\mathbf{x}_k, \boldsymbol{\theta}^*), \frac{1}{2}\right)$$
$$\text{subject to } \boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}(f(\mathbf{x}_k, \boldsymbol{\theta}), \mathbb{1}_{y_k \geq \varepsilon})$$

Differently from regression, the threshold ε appears in both the classification and threshold optimization problems, so they cannot be decomposed.

Black-box optimization Optimization approach based on brute-force.

Black-box optimization

For this problem, black-box optimization can be done as follows:

1. Over the possible values of ε:
   a) Determine the ground truth based on ε.
   b) Train the classifier.
   c) Compute the cost.

Remark. Black-box optimization with grid-search is very costly.

Bayesian surrogate-based optimization Class of approaches to optimize a black-box function f under trivial constraints. It is assumed that f is expensive to evaluate and a surrogate model (i.e., a proxy function) is instead used to optimize it.

Bayesian surrogate-based optimization

Formally, Gaussian surrogate-based optimization solves problems in the form:

$$\min_{x \in B} f(x)$$

where B is a box (i.e., hypercube). f is optimized through a surrogate model $\hat{f}$ that is trained on some observations from f (prior). At each iteration, an acquisition function that uses $\hat{f}$ is used to determine a new point to explore and evaluate with f. The newly discovered sample (posterior) is used to improve $\hat{f}$ and the process is repeated.

Remark. Under the correct assumptions, the result is optimal.

Gaussian process surrogate A good surrogate model should be able to accurately approximate all available training samples and provide a prediction confidence.

A Gaussian process has these properties and can be used as surrogate model.

Acquisition function Function to determine which point to explore next. It should account for both predictions and confidence.

> **Remark.** Acquisition functions should balance exploration (i.e., area with low predictions) and exploitation (i.e., area with high confidence).

Lower confidence bound Acquisition function defined as:

$$\texttt{LCB}(x) = \mu(x) - Z_\alpha \sigma(x)$$

where $\mu(x)$ and $\sigma(x)$ are the predicted mean and standard deviation, respectively. Z_α is a multiplier for the confidence interval.

Given a set of training samples $\{x_i, y_i\}$ and a black-box function f, surrogate-based optimization does the following:

1. Until a termination condition is not met:
   a) Train a surrogate model $\hat{f}$ on $\{x_i, y_i\}$ to approximate f.
   b) Optimize an acquisition function $a_{\hat{f}}(x)$ to find the next data point x' to explore.
   c) Evaluate x' with the black-box function $y' = f(x')$.
   d) Store y' if it is the current best optimum for f.
   e) Add (x', y') to the training set.

5.2.3 Survival analysis (regression)

> **Remark.** Chronologically, this approach has been presented after Chapter 7.

Survival analysis model Probabilistic model to estimate the survival time of an entity.

Survival analysis model

Survival analysis formalization Consider a random variable T to model the survival time. The simplest model can be defined as:

$$t \sim \mathcal{P}(T)$$

Remaining survival time depends on the time $\bar{t}$, therefore we have that:

$$t \sim \mathcal{P}(T \mid \bar{t})$$

Remaining survival time also depends on the past sensor readings $X_{\leq \bar{t}}$ and future readings $X_{>\bar{t}}$ (at this stage, we want to capture what affects the survival time, even if we do not have access to some variables), therefore we have that:

$$t \sim \mathcal{P}\left(T \mid \bar{t}, X_{\leq \bar{t}}, X_{>\bar{t}}\right)$$

Marginalization Average over all the possible outcomes of a random variable to cancel it out.

For this problem, we do not have access to the future sensor readings, so we can marginalize them:

$$t = \mathop{\mathbb{E}}_{X_{>\bar{t}} \sim \mathcal{P}(X_{>\bar{t}})} \left[\mathcal{P}\left(T \mid \bar{t}, X_{\leq \bar{t}}\right)\right]$$

Remark. In probabilistic terms, the regression approach previously taken can be modelled as:

$$t \sim \mathcal{N}(\mu(X_{\bar{t}}), \sigma)$$

where $\mu(\cdot)$ is the regressor.
Compared to the survival analysis model, there are the following differences:

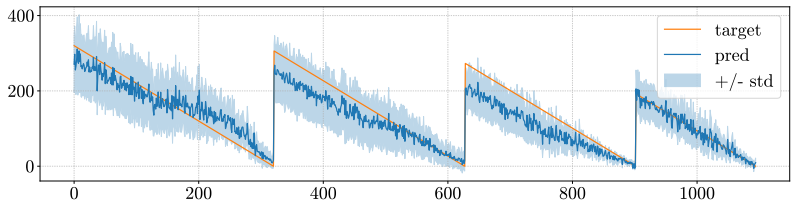
- Regressor only reasons on the sensor readings $X_{\bar{t}}$ at a single time step.
- Regressor does not consider the current time.
- Regressor assumes normal distribution with constant variance.

Neuro-probabilistic model We can assume that the model follows a normal distribution parametrized on both the mean and standard deviation:

$$t \sim \mathcal{N}(\mu(X_{\bar{t}}, \bar{t}), \sigma(X_{\bar{t}}, \bar{t}))$$

Remark. The readings of a single time step are used as it can be shown that using multiple time steps does not yield significant improvements for this dataset.

Architecture Use a neural network that output both μ and σ that are passed to a distribution head.



5.2.4 Survival analysis (classification)

Censoring Hide key events from the dataset. Censoring

Remark. For this dataset, it is more realistic to have more partial runs than run-to-failure experiments as they are expensive to obtain.

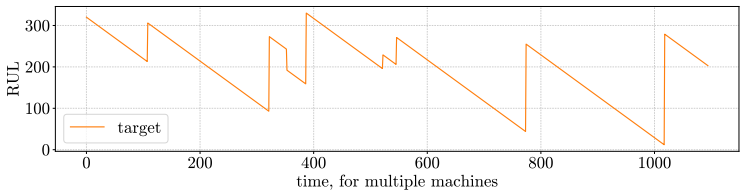


Figure 5.4: Example of partial runs

Survival function Given the random variable T to model survival time, the survival function S is defined as: Survival function

$$S(\bar{t}) = \mathcal{P}\left(T > \bar{t}\right)$$

In other words, it is the probability of surviving at least until time $\bar{t}$.

For this problem, the survival function can account for past sensor readings $X_{\leq \bar{t}}$:

$$S(\bar{t}, X_{\leq \bar{t}}) = \mathcal{P}\left(T > \bar{t} \mid X_{\leq \bar{t}}\right)$$

Hazard function Given the random variable T to model survival time, the hazard function λ is defined as:

$$\lambda(\bar{t}) = \mathcal{P}\left(T < \bar{t} \mid T > \bar{t} - 1\right)$$

In other words, it is the conditional probability of not surviving at time $\bar{t}$ knowing that the entity survived until time $\bar{t} - 1$.

With discrete time, the survival function can be factorized using the hazard function:

$$S(\bar{t}) \approx (1 - \lambda(\bar{t})) \cdot (1 - \lambda(\bar{t} - 1)) \cdot \dots$$

Remark. The hazard function only depends on one observation.

Remark. The fact that the probability of not surviving is used is for historical reasons.

For this problem, the hazard function is the following:

$$\lambda(\bar{t}, X_{\bar{t}}) = \mathcal{P}\left(T < \bar{t} \mid T > \bar{t} - 1, X_{\bar{t}}\right)$$
$$S(\bar{t}, X_{\bar{t}}) \approx (1 - \lambda(\bar{t}, X_{\bar{t}})) \cdot (1 - \lambda(\bar{t} - 1, X_{\bar{t}-1})) \cdot \dots$$

Hazard estimator We want to train an estimator $\hat{\lambda}_\theta(\bar{t}, x_{\bar{t}})$ for the hazard function.

Consider the k-th experiment that ended at time $e^{(k)}$. The probability of the survival event can be modelled as follows:

$$\underbrace{\hat{\lambda}_\theta(e^{(k)}, x^{(k)}_{e^{(k)}})}_{\text{Not surviving at time } e^{(k)}} \underbrace{\prod_{t=1}^{e^{(k)}-1} (1 - \hat{\lambda}_\theta(t, x^{(k)}_t))}_{\text{Surviving until time } e^{(k)} - 1}$$

Training In likelihood maximization terms, the problem for m experiments is formulated as:

$$\arg\max_\theta \prod_{k=1}^{m} \left(\hat{\lambda}_\theta(e^{(k)}, x^{(k)}_{e^{(k)}}) \prod_{t=1}^{e^{(k)}-1} (1 - \hat{\lambda}_\theta(t, x^{(k)}_t)) \right)$$

Let $d^{(k)}_t = 1 \iff t = e^{(k)}$ (i.e., 1 when not surviving at time t), the problem can be rewritten as:

$$\begin{aligned}
&\arg\max_\theta \prod_{k=1}^{m} \prod_{t=1}^{e^{(k)}} d^{(k)}_t \hat{\lambda}_\theta(t, x^{(k)}_t) + (1 - d^{(k)}_t)(1 - \hat{\lambda}_\theta(t, x^{(k)}_t)) \\
&= \arg\max_\theta \sum_{k=1}^{m} \sum_{t=1}^{e^{(k)}} \log\left(d^{(k)}_t \hat{\lambda}_\theta(t, x^{(k)}_t) + (1 - d^{(k)}_t)(1 - \hat{\lambda}_\theta(t, x^{(k)}_t)) \right) \\
&= \arg\max_\theta \sum_{k=1}^{m} \sum_{t=1}^{e^{(k)}} d^{(k)}_t \log\left(\hat{\lambda}_\theta(t, x^{(k)}_t) \right) + (1 - d^{(k)}_t) \log\left(1 - \hat{\lambda}_\theta(t, x^{(k)}_t) \right) \\
&= \arg\min_\theta - \sum_{k=1}^{m} \sum_{t=1}^{e^{(k)}} d^{(k)}_t \log\left(\hat{\lambda}_\theta(t, x^{(k)}_t) \right) + (1 - d^{(k)}_t) \log\left(1 - \hat{\lambda}_\theta(t, x^{(k)}_t) \right)
\end{aligned}$$

Which corresponds to a binary cross-entropy minimization problem where $d^{(k)}_t$ can be seen as the class. Therefore, $\hat{\lambda}_\theta(t, x^{(k)}_t)$ can be seen as a classifier.

Remark. This shows that the classification approach used in Section 5.2.2 is not strictly wrong. Instead of predicting whether the machine fails in ε time steps, in probabilistic terms, the correct approach is to consider whether the machine fails at a time step t knowing it survived at time $t-1$.

Remark. Censored data skews the distribution of the data. Sample weights can be used to deal with the issue.

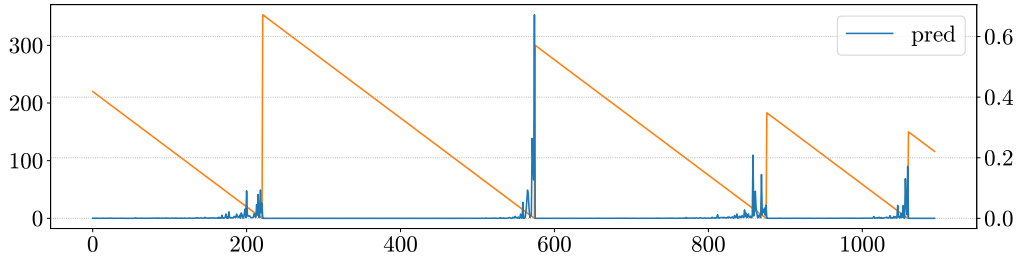


Figure 5.5: Failure probability of the classifier

Inference Given a threshold ε, maintenance is triggered when:

$$\hat{\lambda}(t, x_t) \geq \varepsilon$$

Forecasting Determine the probability of surviving n more steps as:

$$\begin{aligned}\frac{S(t+n)}{S(t)} &= \prod_{h=0}^{n}(1-\lambda(t+h, X_{t+h})) \\ &\approx \prod_{h=0}^{n}(1-\hat{\lambda}(t+h, x_{t+h}^{(k)}))\end{aligned}$$

However, this would require accessing future values of X_t. Possible workarounds are:

- Ignore time-varying inputs (i.e., sort of marginalization) so that $\hat{\lambda}(t+h, x_{t+h}) \approx \hat{\lambda}(t+h, x^{(k)})$ where $x^{(k)}$ only contains stable information.
- Predict future values of $x_t^{(k)}$ by training another estimator.
- Assume that all the variables $x_t^{(k)}$ are stable for some time so that:

$$\frac{S(t+n)}{S(t)} \approx \prod_{h=0}^{n}(1-\hat{\lambda}(t+h, x_t^{(k)}))$$

6 Component wear anomalies: Skin wrapper machines

6.1 Data

The dataset represents a single run-to-failure experiment of a skin wrapper machine with a 4 ms sampling period and different segments (i.e., operating mode).

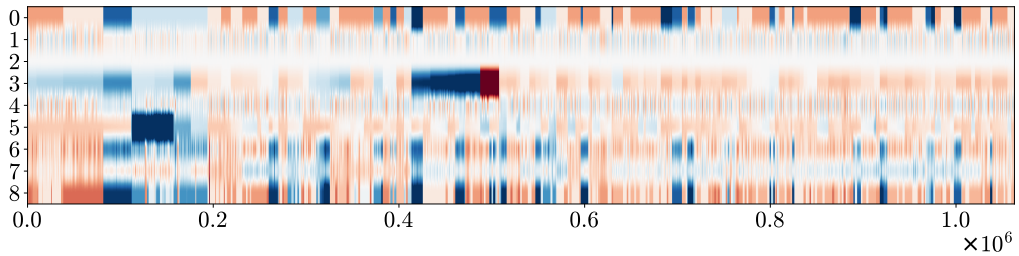
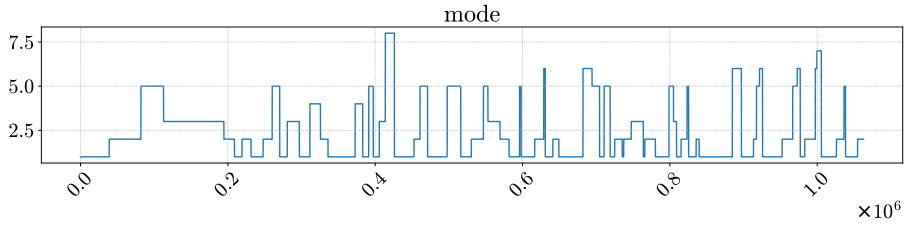


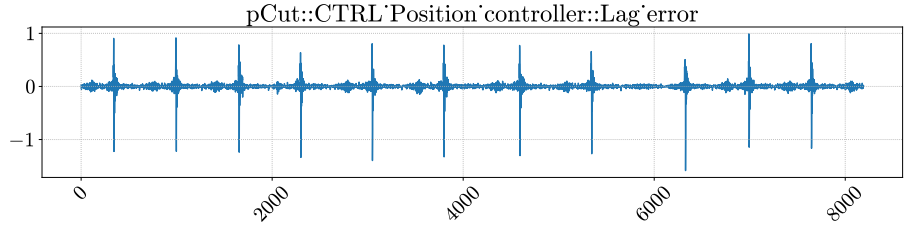
Figure 6.1: Dataset heatmap

The following observations can be made:

- Some features (i.e., rows 0 and 8 of the heatmap) are fixed for long periods of time (i.e., piece-wise constant). They are most likely controlled parameters.

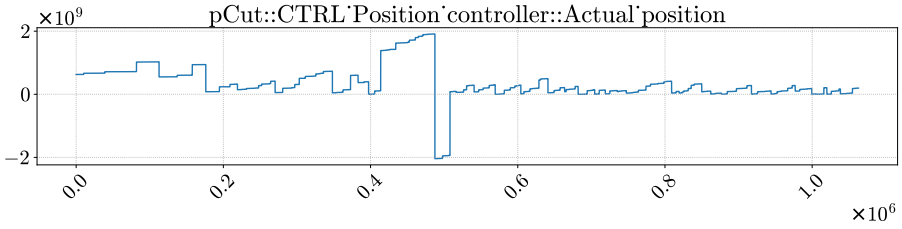


- A feature (i.e., row 2 of the heatmap) seems constant but in reality it has many short-lived peaks.



| **Remark.** This type of signal might be useful to determine a period in the series.

- Some features (i.e., rows 3 and 5 of the heatmap) contain sudden localized deviations. This is most likely due to external interventions.



6.1.1 Binning

Binning Reduce the granularity of the data using a non-overlapping sliding window and aggregation functions. Binning

> **Remark.** With high-frequency data, some approaches (e.g., a neural network) might not be able to keep up if real-time predictions are required.

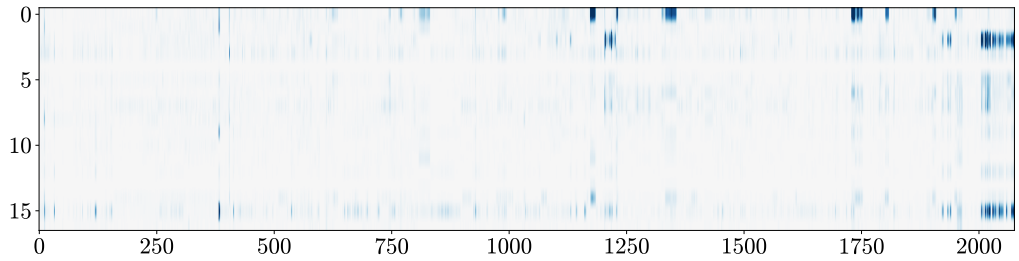
> **Remark.** After binning, the number of samples is reduced, but the number of features might increase.

6.2 Approaches

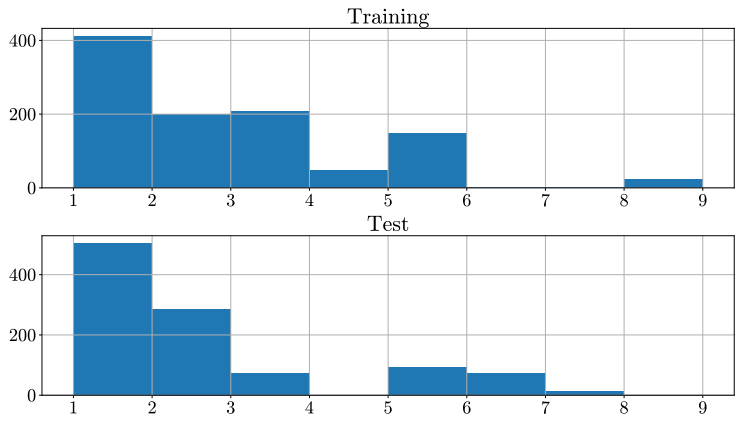
6.2.1 Autoencoder

Autoencoder Train an autoencoder on earlier non-anomalous data and use the reconstruction error to detect component wear.

Results show that there is a high reconstruction error for the operating mode feature (i.e., first row), which is a controlled parameter. This hints at the fact that some operating modes are too infrequent, so the model is unable to reconstruct them.



> **Remark.** There is a distribution drift (i.e., future does not behave like the past) in the dataset.



Remark. To account for distribution drift, chronological splitting for the training and test sets is a better approach instead of random sampling (which ignores the drift).
The validation set can be created through random sampling as, in case it is created chronologically, it might create a gap between training and test data. However, this approach ignores drift when validating.

6.2.2 Class rebalancing

Remark. Consider two training samples $\{(x_1, y_1), (x_2, y_2)\}$, the optimization problem over an objective function f_θ would be:

$$\arg\max_\theta f_\theta(y_1|x_1) f_\theta(y_2|x_2)$$

If the second sample (x_2, y_2) appears twice, the problem is:

$$\begin{aligned}&\arg\max_\theta f_\theta(y_1|x_1) f_\theta(y_2|x_2)^2 \\ &= \arg\max_\theta f_\theta(y_1|x_1)^{\frac{1}{3}} f_\theta(y_2|x_2)^{\frac{2}{3}}\end{aligned}$$

Importance sampling Given an empirical risk minimization problem: Importance sampling

$$\arg\min_\theta -\prod_{i=1}^{m} f_\theta(y_i|x_i)$$

Each training sample can have associated a different weight w_i:

$$\begin{aligned}&\arg\min_\theta -\prod_{i=1}^{m} f_\theta(y_i|x_i)^{w_i} \\ &= \arg\min_\theta -\sum_{i=1}^{m} w_i \log\left(f_\theta(y_i|x_i)\right)\end{aligned}$$

The weights can be seen as a ratio:

$$w_i = \frac{p_i^*}{p_i}$$

where:

- p_i is the sampling bias that has to be canceled out.
- p_i^* is the target distribution to emulate.

In this problem, we can define the weights as follows:

$$\begin{aligned}p_i &= \frac{1}{n}|\text{samples with the same operating mode as } x_i| \\ p_i^* &= \frac{1}{n}\end{aligned}$$

Remark. As uniform distribution is assumed, the detector will not be sensitive to the mode.

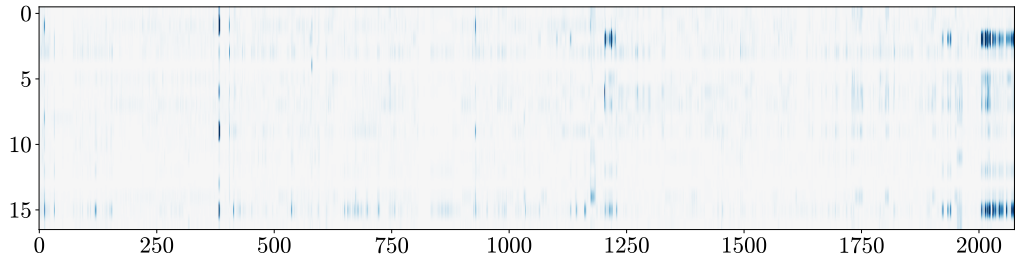


Figure 6.2: Autoencoder feature reconstruction error with importance sampling. Note that the operation mode (row 0) now has fewer errors.

6.2.2.1 Importance sampling applications

Class rebalancing Oversample or undersample training samples based on the class unbalance.

> **Remark.** When evaluating a model trained on a rebalanced training set, accuracy might not be the ideal metric. A cost model or confusion matrix can be used.

> **Remark.** Rebalancing should not be used when the data is unbalanced but representative of the real distribution.

Remove bias from continuous attributes p_i and p_i^* can be probability densities. Therefore, with a continuous feature, it is sufficient to estimate p_i using a density estimator.

> **Remark.** It can be useful to clip p_i for numerical stability:
>
> $$p_i = \max(l, \min(u, f(x_i, y_i)))$$

Remove bias from external attributes If the dataset is generated from biased external sources, it is possible to attempt to debias it by determining the probability that a sample belong to the dataset and use it as p_i.

> **Example.** A dataset for organ transplants already contains patients for which doctors think the surgery is more likely to be successful.
> p_i can be the probability that the patient has been selected to be an organ receiver.

Sample-specific variance Importance sampling applied with MSE allows to remove its homoscedasticity (i.e., allow non-constant variance).

Consider MSE formulated as follows:

$$\arg\min_\theta -\sum_{i=i}^{m} \log\left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(y_i - h_\theta(x_i))^2\right)\right)$$

By adding as weights $\frac{1}{\hat{\sigma}_i^2}$, the problem becomes:

$$\begin{aligned}
&\arg\min_\theta -\sum_{i=i}^{m} \frac{1}{\hat{\sigma}_i^2} \log\left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(y_i - h_\theta(x_i))^2\right)\right) \\
&= \arg\min_\theta -\sum_{i=i}^{m} \log\left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y_i - h_\theta(x_i))^2}{2\hat{\sigma}_i^2}\right)\right)
\end{aligned}$$

In other words, the weight in the form $\frac{1}{\hat{\sigma}_i^2}$ represents the inverse sample variance. Therefore, it is possible to specify a different variance for each sample.

7 Arrivals prediction: Hospital emergency room

7.1 Data

The dataset contains accesses to the emergency room of the Maggiore Hospital in Bologna. Each row of the dataset represents a patient and the features are:

`Triage` Time of arrival.

`TKCharge` Time of first visit.

`Code` Priority (`white`, `green`, `yellow`, and `red`).

`Outcome` Indicates whether the patient got admitted or left.

Binning As the problem is to predict the total number of arrivals at fixed intervals, binning can be used to obtain a dataset with an hour granularity.

7.2 Approaches

Remark. MSE assumes that the conditional distribution $\mathcal{P}(y|x;\theta)$ of the predictions follows a normal distribution (i.e., $y \sim \mathcal{N}(\mu(x;\theta), \sigma)$).

Remark. Arrivals usually follow a Poisson distribution as:

- There is a skew in the tail.
- All values are positive.
- Events are independent.

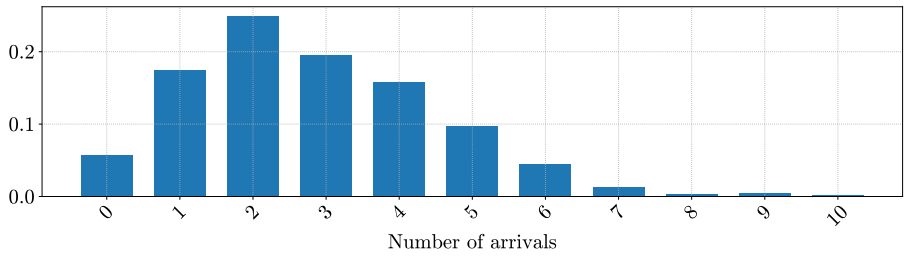


Figure 7.1: Arrivals distribution at 6 a.m.

Theorem 7.2.1. If the inter-arrival time is exponential with respect to a fixed rate, the counts of the arrivals will always follow a Poisson distribution.

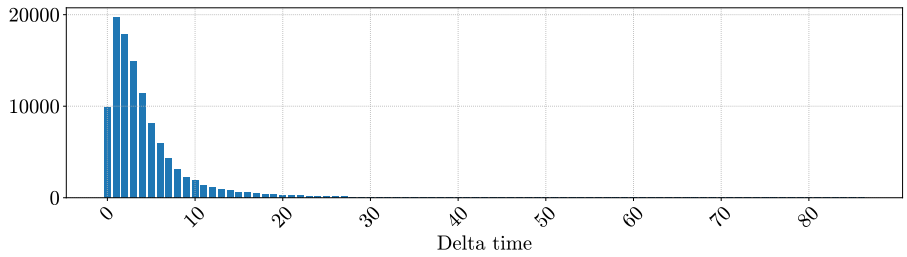


Figure 7.2: Dataset inter-arrival counts (the first bar is due to binning artifacts)

7.2.1 Neuro-probabilistic model

Poisson distribution

Poisson distribution Distribution with discrete support whose probability mass function is defined as:

$$p(k, \lambda) = \frac{\lambda^k e^{-\lambda}}{k!}$$

where λ is the occurrence rate of the events.

Remark. Both mean and standard deviation of a Poisson distribution are λ.

Remark. $\lambda^{-\frac{1}{2}}$ represent the distribution skewness. For smaller values of λ, there is a positive skew to the left. For larger values of λ, the skew becomes less observable.

Remark. For this problem, λ is the average number of arrivals in each bin.

Neuro-probabilistic model

Neuro-probabilistic model Model that combines statistics and machine learning.

Remark. This class of models is known in the statistics literature as generalized linear model. With neural networks (i.e., non-linearity), they do not have an official name. "Neuro-probabilistic model" is an unofficial name.

This problem can be formulated through the following probabilistic model:

$$y \sim \texttt{Poisson}(\lambda(x))$$

where y is the number of arrivals and $\lambda(x)$ is the rate parametrized on the temporal information x.

The rate can be approximated using an estimator as:

$$y \sim \texttt{Poisson}(\lambda(x, \theta))$$

where $\lambda(x, \theta)$ is a regression model.

Loss Training is done for maximum likelihood estimation using the Poisson distribution:

$$\begin{aligned} &\arg\min_\theta - \sum_{i=1}^{m} \log\left(f(y_i, \lambda(x_i, \theta))\right) \\ &= \arg\min_\theta - \sum_{i=1}^{m} \log\left(\frac{\lambda(x_i, \theta)^{y_i} e^{\lambda(x_i, \theta)}}{y_i!}\right) \end{aligned}$$

Architecture Use an MLP to predict $\hat{\lambda}$ and then, instead of outputting the prediction directly, output a Poisson distribution object with rate $\hat{\lambda}$:

$$\begin{aligned} \hat{\lambda} &= \texttt{MLP}(x) \\ \texttt{out} &= \texttt{Poisson}(\cdot, \hat{\lambda}) \end{aligned}$$

Some considerations must be made:

Only positive rates As $\hat{\lambda}$ must be positive, it is possible to combine a logarithm (i.e., assume that the MLP outputs a log-rate) and an exponentiation to achieve this:

$$\begin{aligned}\log(\hat{\lambda}) &= \texttt{MLP}(x)\\ \texttt{out} &= \texttt{Poisson}\left(\cdot, \exp\left(\log(\hat{\lambda})\right)\right) = \texttt{Poisson}(\cdot, \hat{\lambda})\end{aligned}$$

Remark. A strictly positive activation function can also be used.

Standardization The input of the network can be standardized. On the other hand, standardizing the output is wrong as the Poisson distribution is discrete.

However, if the input is standardized (for training stability), the output of the network with normal weights initialization will have 0 mean. Therefore, at the beginning, the network will predict $\hat{\lambda} \approx 1$ (i.e., the MLP predicts $\log(\hat{\lambda}) \approx 0$ and then $\hat{\lambda} = \exp\left(\log(\hat{\lambda})\right) \approx 1$) which might not be a reasonable starting point.

It is possible to provide an initial guess $\bar{\lambda}$ for $\hat{\lambda}$. This value can be used as a multiplicative factor, so that the first prediction will be close to $\bar{\lambda} \cdot 1$:

$$\begin{aligned}\log(\hat{\lambda}) &= \texttt{MLP}(x)\\ \texttt{out} &= \texttt{Poisson}\left(\cdot, \bar{\lambda}\exp\left(\log(\hat{\lambda})\right)\right) = \texttt{Poisson}(\cdot, \bar{\lambda}\hat{\lambda})\end{aligned}$$

Remark. For this problem $\bar{\lambda}$ can be the average number of arrivals in each bin.

Remark. With one-hot encoding, a linear model can be non-linearized into a lookup table.

Example.

Consider the dataset:

x	y
0	1
1	4
2	2

A linear model learns a straight line:

$$f(x) = \alpha x$$

With the dataset:

x_0	x_1	x_2	y
1	0	0	1
0	1	0	4
0	0	1	2

A linear model learns a linear combination:

$$f(x) = \alpha x_0 + \beta x_1 + \gamma x_2$$

Which allows to easily learn the dataset with $\alpha = 1$, $\beta = 4$, and $\gamma = 2$

Remark. Having access to the distribution allows to compute all possible statistics. For instance, it is possible to plot mean and standard deviation.

8 Feature selection and important: Biomedical analysis

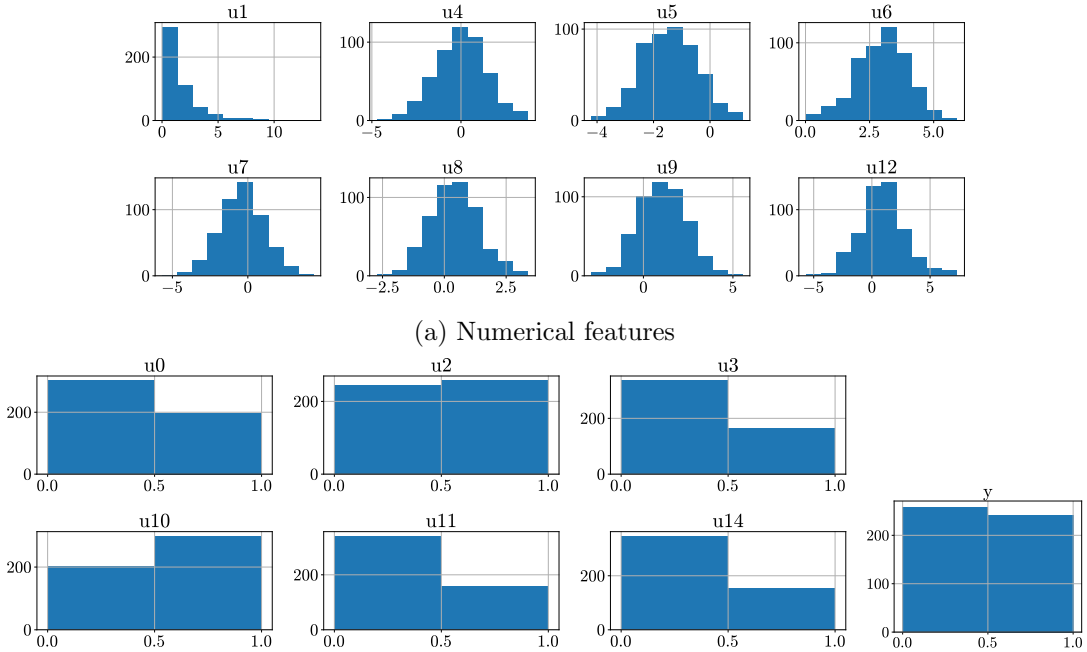
8.1 Data

The dataset contains anonymized biomedical data and is composed of a binary target variable and unknown variables.

Remark. In reality, this dataset contains real-world examples. Features have been anonymized for the purpose of feature analysis.

8.1.1 Preliminary analysis

Data distribution There are both categorical and numerical features.



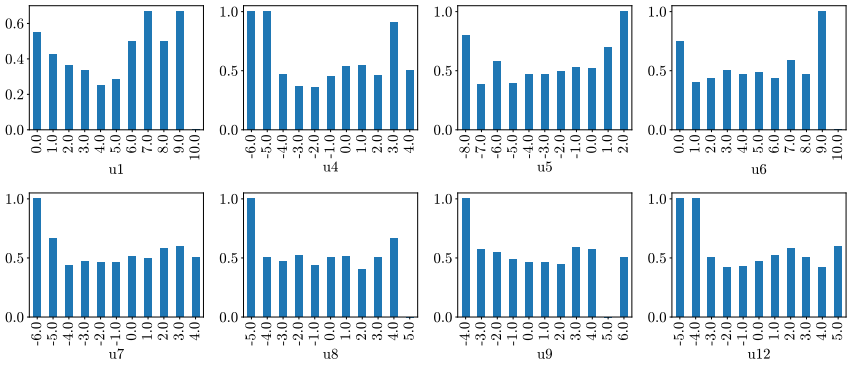
(a) Numerical features

(b) Categorical features

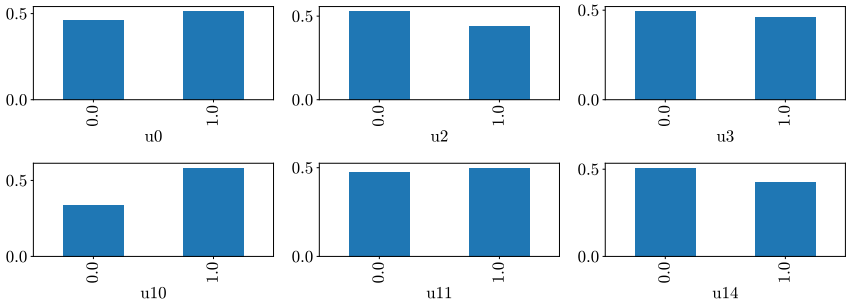
(c) Target

Figure 8.1: Distribution of the dataset

Univariate dependencies Determine the fraction of examples with target $Y = 1$ (i.e., likelihood that a feature has a specific value while the target is 1).



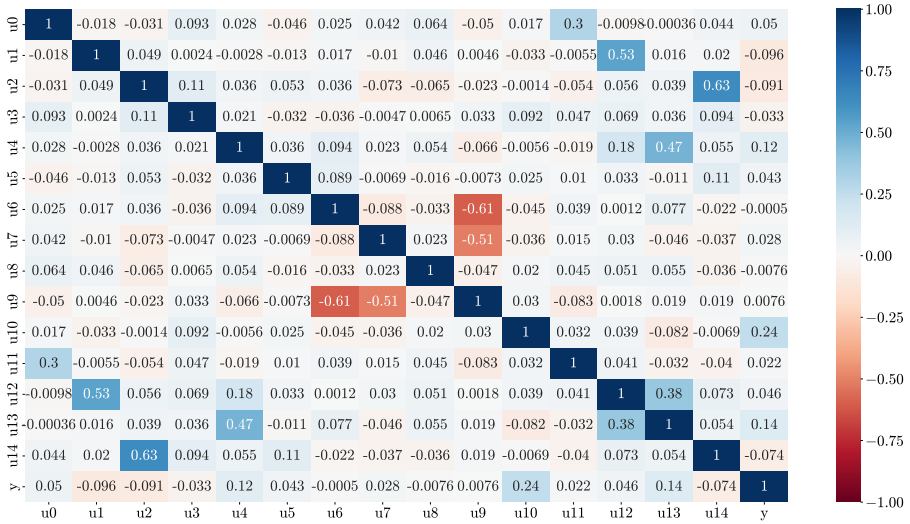
(a) Numerical features



(b) Categorical features

Figure 8.2: Univariate dependencies with $Y = 1$

Linear correlation Determine the Pearson's correlation between variables.



8.2 Approaches

8.2.1 Linear model

Linear model for explanation Use a linear model (logistic regression in this case) as a proxy to explain the features.

Linear model for explanation

Remark. Preventing overfitting is important as the model has to generalize well. L1 regularization ($\alpha\|\boldsymbol{\theta}\|_1$) can help by:

- Preventing overfitting.
- Sparsifying the coefficients (i.e., make them mostly close to 0). The hyperparameter α controls this behavior.

  Example. Consider the case of MSE with L1 regularization. The gradient of L1 is never 0 and is upper-bounded whereas the gradient of MSE can be 0 and can go to ∞. This produces the following phenomenon:

  – When close to 0, the slope of ∇`MSE` is larger and outweighs ∇`L1`, making updates follow MSE.

  – When moving away from 0, ∇`MSE` becomes smaller up to a point where it balances with ∇`L1`. At this point, updating that parameter does not improve the loss anymore.

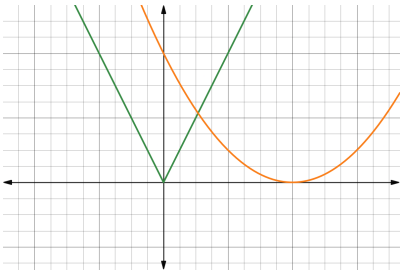


Figure 8.3: MSE (orange) and L1 (green)

Remark. ROC-AUC is a good metric for non-deterministic classification problems. While accuracy is more suited for deterministic approaches.

Coefficient analysis By using a linear model, its coefficients can be analyzed to determine the weights of the features.

Remark. For the weights to make sense, it is important to normalize the features.

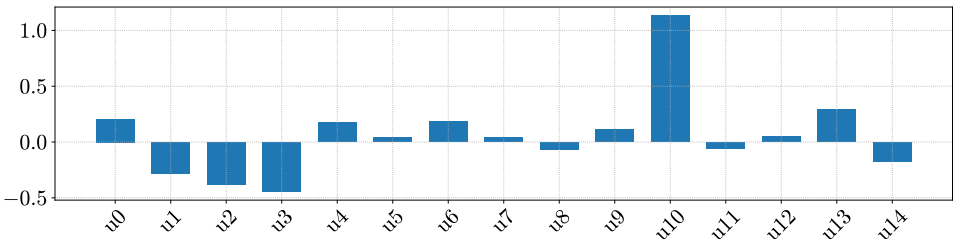


Figure 8.4: Coefficients for this problem

Issues A linear model has several limitations for explainability:

- Being linear, it might not have good performance on the training data. Therefore, feature analysis might not be accurate.
- Only linear correlations can be captured.

- Coefficients are not necessarily sparse as L1 has to balance between sparsification and overfitting.

Remark. A linear model approach is similar to using the correlation matrix. The only difference is that:

- Pearson's coefficient is computed between a pair of variables.
- A linear model considers all the variables at once.

8.2.2 Non-linear model

Non-linear model for explanation Use a non-linear model (gradient boosted trees in this case) as a proxy to explain the features.

Non-linear model for explanation

Remark. Compared to linear models, non-linear models might have better performance but are less explainable and risks overfitting.

Features importance analysis By using trees, feature importances can be computed.

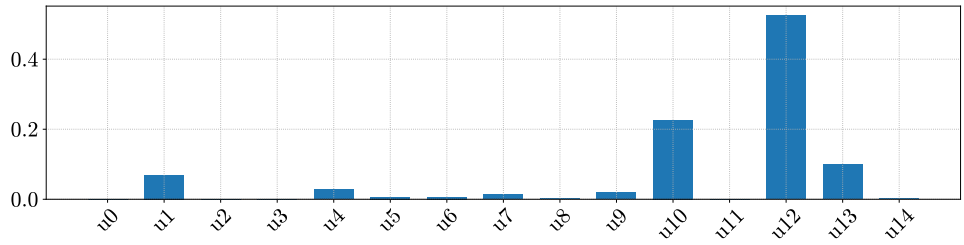


Figure 8.5: Feature importances (gain) for this problem

Remark. Feature importance can be computed using different metrics which will not necessarily produce the same results. Some possible metrics are:

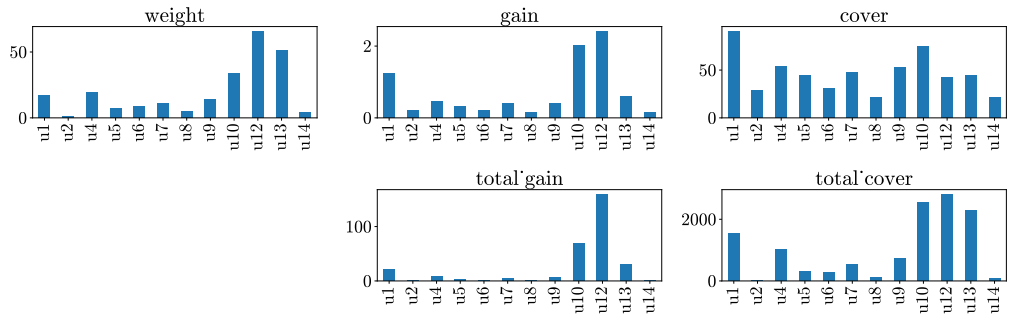
Weight The number of times a feature has been used to split.

Gain Average gain from the splits of a feature.

Cover Average number of examples for which a feature is used as decision criteria.

Total gain Sum of the gains from the splits of a feature.

Total cover Sum of the number of examples for which a feature is used as decision criteria.



Moreover, feature importances are associated with the training data. Therefore, it risks overfitting.

Permutation importance analysis Given:

- A trained model,
- An evaluation metric,
- A reference dataset $\{x_i, y_i\}_{i=1}^m$.

Permutation importance for the j-th feature is computed by randomly permuting the j-th column in the dataset and computing the difference between the performance on the original and permuted dataset.

For more statistical relevance (i.e., remove spurious correlations), the process can be repeated multiple times and presented using mean and standard deviation.

Remark. Permuting the values of a feature aims at preserving the distribution of the column while breaking all correlations.

Remark. This approach works on black box models. However, it tends to be expensive.

Remark. If the reference dataset is the training set, permutation importance can be used to determine how the model is using the data. On the other hand, by using the test set, the scores will reflect the correlation between the attributes and the target.

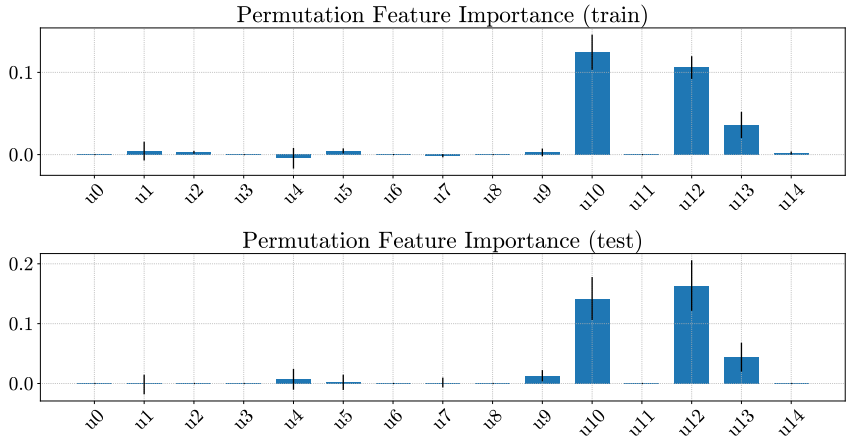


Figure 8.6: Permutation importance on train and test set. u_{10} is slightly higher on the train set, which indicates that it might be causing a bit of overfitting.

Remark. Compared to linear models, non-linear models do not have the capability of identifying the direction of correlation.

8.2.3 Additive feature attribution

Linear models Given a linear model, an individual example $\mathbf{x}$ can be explained using an additive attribution model as the difference between the prediction and average prediction over the distribution:

$$\boldsymbol{\theta}^T\mathbf{x} - \mathbb{E}_{\mathbf{x}' \in P(\boldsymbol{X})}\left[\boldsymbol{\theta}^T\mathbf{x}'\right]$$

$\mathbb{E}_{\mathbf{x}' \in P(X)}\left[\boldsymbol{\theta}^T\mathbf{x}'\right]$ can be approximated as the average prediction on the training data and it represents the prediction that the model would make if no information is provided.

Due to linearity, the formula can be rewritten as follows:

$$\begin{aligned}\boldsymbol{\theta}^T\mathbf{x} - \mathbb{E}_{\mathbf{x}'\in P(\boldsymbol{X})}\left[\boldsymbol{\theta}^T\mathbf{x}'\right] &= \boldsymbol{\theta}^T(\mathbf{x} - \mathbb{E}_{\mathbf{x}'\in P(\boldsymbol{X})}\left[\mathbf{x}'\right]) \\ &= \sum_{j=1}^{n}\boldsymbol{\theta}_j(\mathbf{x}_j - \mathbb{E}_{\mathbf{x}'\in P(\boldsymbol{X})}\left[\mathbf{x}'_j\right]) \\ &= \sum_{j=1}^{n}\phi_j(\mathbf{x})\end{aligned}$$

where $\phi_j(\mathbf{x}) = \boldsymbol{\theta}_j(\mathbf{x}_j - \mathbb{E}_{\mathbf{x}'\in P(\boldsymbol{X})}[\mathbf{x}'_j])$ is the **effect** of the j-th attribute on the output for the example $\mathbf{x}$ (i.e., how much it moves from the baseline prediction). Effect

Non-linear models Given a non-linear model, an example $\mathbf{x}$ can be explained using an additive attribution model defined as follows:

$$g(\mathbf{z}, \mathbf{x}) = \phi_0 + \sum_{j=1}^{n}\phi_j(\mathbf{x})\mathbf{z}_j$$

where:

- ϕ_0 is the baseline prediction (i.e., average prediction over the dataset).
- ϕ_j is the effect of the j-th feature.
- $\mathbf{z}_j \in \{0, 1\}$ indicates whether the j-th feature is known.

In practice, given an example $\mathbf{x}$ and the flags $\mathbf{z}$, a linear explanation model is trained locally to tune the effect coefficients ϕ_j of $g(\mathbf{z}, \mathbf{x})$.

Shapely values Closed-form formula to determine the effect coefficients. Given the set of all input features $\mathcal{J}$, the Shapely value of the j-th feature is computed as: Shapely values

$$\phi_j(\mathbf{x}) = \sum_{\mathcal{S}\subset\mathcal{J}\setminus j}\frac{|\mathcal{S}|!(n - |\mathcal{S}| - 1)!}{n!}(\hat{f}(\mathbf{x}_{\mathcal{S}\cup j}) - \hat{f}(\mathbf{x}_{\mathcal{S}}))$$

Intuitively, by fixing the j-th attribute, ϕ_j is computed by considering all the possible combinations of the $\mathbf{z}_i$ values of the other attributes (i.e., different subsets $\mathcal{S}$ of the features without j) and averaging the difference between the prediction that uses as features $\mathcal{S} \cup j$ and the baseline that only uses $\mathcal{S}$.

> **Remark.** Shapely values are expensive to compute due to the exponential number of terms. Moreover, many models do not support missing values.

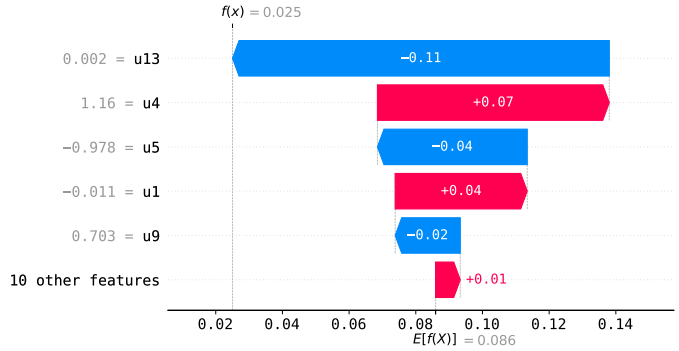
SHAP Framework to approximate Shapely values for black-box models. SHAP

Kernel SHAP Given an example $\mathbf{x}$, kernel SHAP does the following:

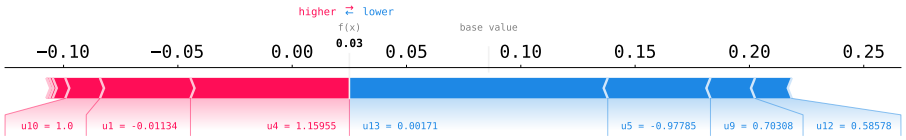
1. Sample multiple $\mathbf{z}'$ vectors from $\{0, 1\}^n$.
2. For every sampled vector, construct an example $\mathbf{x}'$ such that:
   - $\mathbf{x}'_j = \mathbf{x}_j$ if $\mathbf{z}'_j = 1$.
   - $\mathbf{x}'_j$ is sampled from a background set (e.g., training set) if $\mathbf{z}'_j = 0$.
3. Train a linear model on the created examples and determine Shapely values using it.

Plots Shapely values can be visualized through several plots:

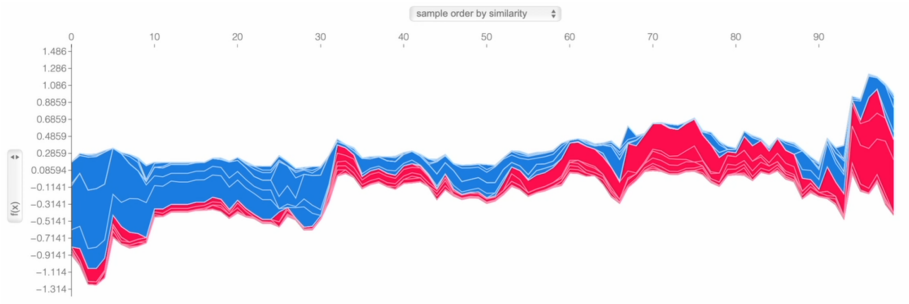
Waterfall plot Shows the most relevant features that allowed to reach the prediction $f(x)$ starting from the baseline $\mathbb{E}[f(x)]$.



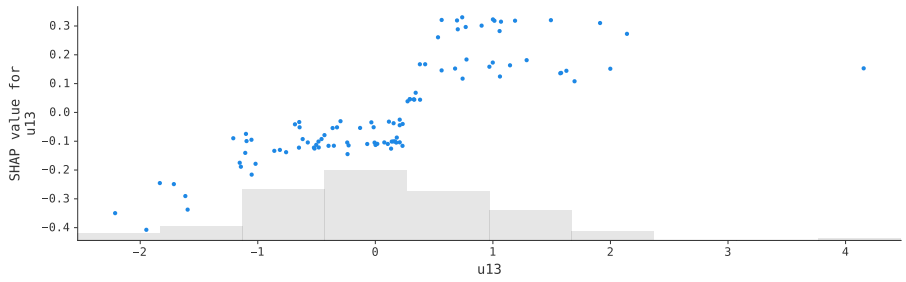
Force plot Compact version of waterfall plots.



Global force plot Stack of force plots where the x-axis represents the examples.

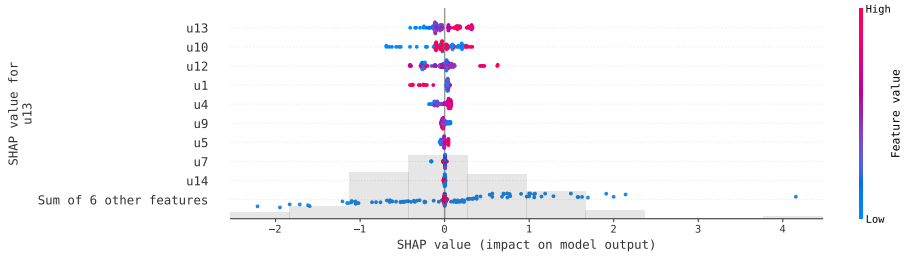


Scatter plot Links the values of an attribute to its Shapely values.



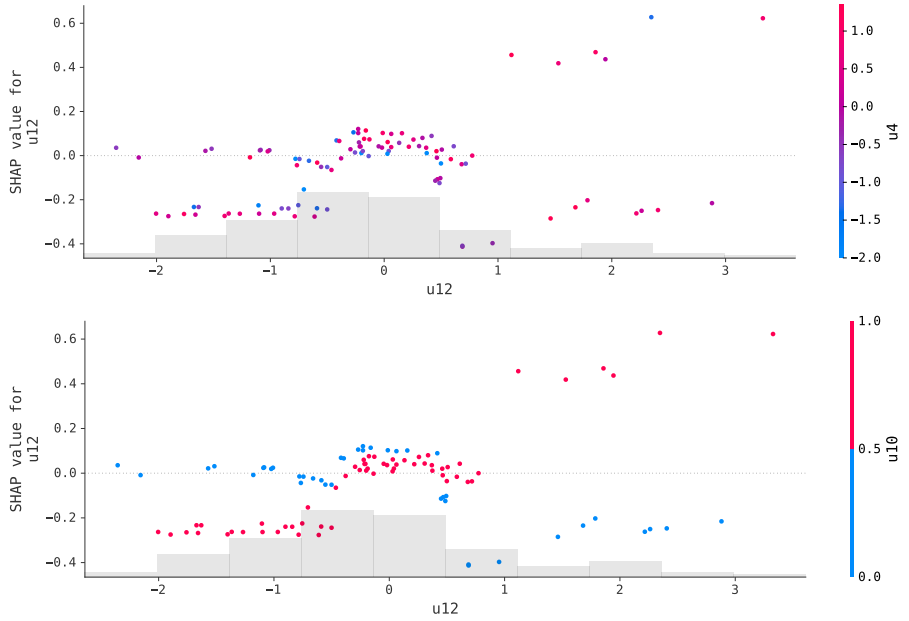
| **Remark.** A growing trend indicates a positive correlation.

Beeswarm summary plot Stack of multiple scatter plots. The values of the attributes are color coded (instead of being at the x-axis).



Remark. A color gradient indicates correlation.

Scatter dependency plot Links the combined effect of two attributes. Starting from the scatter plot of the first attribute, points are colored based on the values of the second attribute.

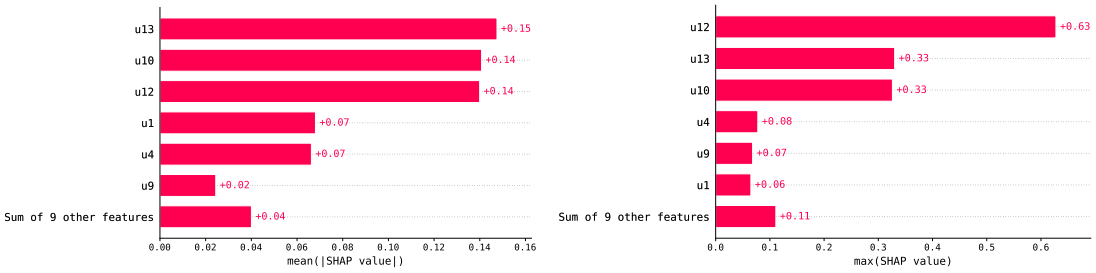


Remark. As is, SHAP does not provide single values (e.g., feature importance) but only values for each example.

Global feature analysis Aggregate local Shapely values to obtain global explanations. For instance, a possible approach is averaging over the examples:

$$\bar{\phi}_j(x) = \frac{1}{n} \sum_{i=1}^{m} |\phi_j(x_i)|$$

Remark. This approach is heuristic. Shapely values have well-defined semantics and the result of aggregation is not clear.



8.2.4 Optimization-oriented feature selection

Optimization-oriented feature selection Given the set of features $\mathcal{J}$, solve the problem: Optimization-oriented feature selection

$$\arg\min_{\mathcal{S}\subseteq\mathcal{J}} \left\{ |\mathcal{S}| : \forall(x,y).\, \hat{y} = \hat{f}_{\mathcal{S}}(x_{\mathcal{S}}), \mathcal{L}(y,\hat{y}) \leq \theta \right\}$$

In other words, this is the problem of determining the smallest subset of features $\mathcal{S}$ such that a model $\hat{f}_{\mathcal{S}}$ trained only considering them has an acceptable performance.

Remark (Pareto fronts)**.** This problem can be solved as a multi-objective optimization problem using Pareto fronts to discard unnecessary points and only consider those that graphically do not have other points in the top-left area above them.

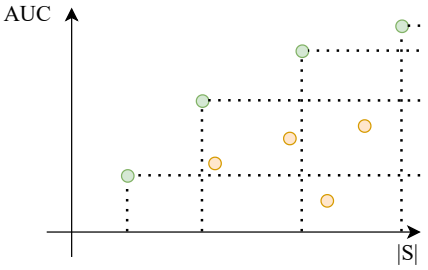


Figure 8.9: Green points are non-dominated and orange points are dominated

Remark. This approach aims at obtaining the best possible performance. Therefore, it is reasonable for a normal machine learning problem. However, for determining features importance, this is not ideal.

8.2.5 Statistical hypothesis testing

Statistical hypothesis testing Given: Statistical hypothesis testing

- A random (possibly multivariate) variable X,
- A hypothesis $H(X)$.

We can define:

- A competing null hypothesis $H_0(X)$,
- An experimental statistics $T[X]$ (e.g., expected value).

Remark. H_0 is often the negation of H and $T[X]$ is a value that supports the hypothesis when large enough.

By assuming that the null hypothesis holds, we need to compute:

- The empirical value $T[x \mid H_0]$.
- The theoretical probability $\mathcal{P}(T[X \mid H_0])$.

p-value Probability $\mathcal{P}(T[X \mid H_0])$ of observing an empirical value as extreme as $\mathcal{P}(T[X])$ under the null hypothesis (e.g., $\mathcal{P}(T[X \mid H_0] \geq t)$ or $\mathcal{P}(T[X \mid H_0] \leq t)$, depending on the case). If $p < 1 - \alpha$, for a given confidence interval α (e.g., 0.95), H_0 is likely false. p-value

Example. For this problem:

- Variables can be feature-target pairs (X, Y).

- The hypothesis can be $H \equiv$ "X is important to predict Y" (following a given correlation score $r[X, Y]$ such as average Shapely value, permutation importance, ...).
- The null hypothesis can be $H_0 \equiv$ "X is important by chance".

Given the correlation score for the original dataset $r^* = r[x, y]$, we can define the following inequality:

$$r[\tilde{x}, \tilde{y}] \leq r^*$$

where $(\tilde{x}, \tilde{y})$ is sampled from $(\tilde{X}, \tilde{Y})$, which is a similar but uncorrelated version of (X, Y). If X and Y are correlated, it is expected that the inequality holds most of the time, otherwise it should be half of the time. Therefore, we can define the test statistics for this problem as:

$$T[X, Y \mid H_0] \equiv \sum_{i=1}^{m} \mathcal{P}\left(r[\tilde{X}, \tilde{Y}] \leq r^*\right)$$

where m is the number of samples drawn from $(\tilde{X}, \tilde{Y})$. If $T[X, Y \mid H_0] \sim \frac{m}{2}$, we can state that X and Y might not be correlated.
The test $r[\tilde{X}, \tilde{Y}] \leq r^*$ has a binary outcome and therefore its theoretical probability follows a Bernoulli distribution (if H_0 holds, it follows $\mathcal{B}(\frac{1}{2})$). If the experiment is repeated n times, the probability of $T[X, Y \mid H_0]$ follows a binomial distribution $\mathcal{B}(n, \frac{1}{2})$.
In practice, to create an uncorrelated dataset $(\tilde{X}, \tilde{Y})$, it is possible to permute the values of a feature in X. Then, it is possible to compute the empirical value $T[X, Y \mid H_0]$ and match it against the theoretical probability. The p-value can be computed as:

$$p = \mathcal{P}\left(T[X, Y \mid H_0] \geq t\right)$$

where t defines a target interval in the distribution and depends on the theoretical distribution and the confidence level α. If $p < 1 - \alpha$, we can reject H_0. To reduce sampling noise, the experiment can be repeated multiple times.

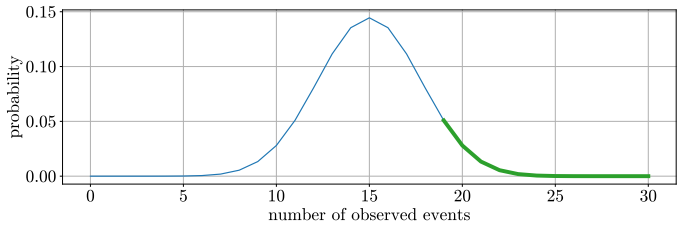


Figure 8.10: Binomial distribution with 30 samples. The interval defined with $\alpha = 0.95$ is in green.

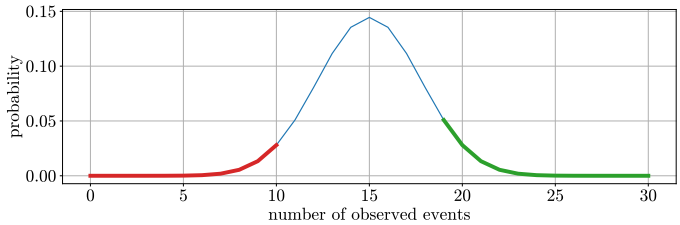
Remark. When $p < 1 - \alpha$, it is possible to reject H_0 and state that H is most likely true. However, in all other cases nothing can be concluded.
With binary hypotheses, it is possible to negate H and repeat the procedure with $\neg H$, allowing to create two target intervals to have more information.

Example. For this case, we have that:

- The negated hypothesis is $\neg H \equiv$ "X is not important to predict Y".
- H_0 remains the same.
- The test statistics becomes $n - T[X, Y \mid H_0]$.

By proceeding as before, we can ultimately obtain the following intervals:

- One that supports H.
- One that supports $\neg H$.
- One where no claim can be made.



Boruta Algorithm for feature selection based on statistical hypothesis testing with the hypothesis $H \equiv$ "feature j is important among those in the dataset according to a given metric" Boruta

Given a dataset (X, Y), Boruta works as follows:

1. Augment the dataset with a permuted version $\tilde{X}_j$ of each feature (shadow features).
2. Run the statistical test based on:

$$\phi_j((x, \tilde{x}), y) > \max_{j \in \tilde{X}} \phi_j((x, \tilde{x}), y)$$

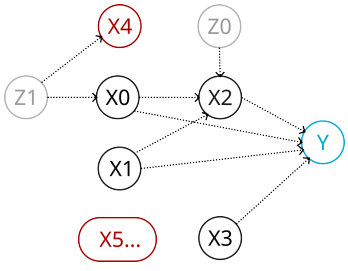
   where ϕ is a feature importance metric (e.g., obtained from decision trees). Intuitively, the importance of a feature j is compared with the importances of the shadow features.
3. Repeat the experiment multiple times.

Remark. Due to the maximum operation, the theoretical distribution of T is mostly binomial. So, some statistical corrections are applied.

Remark. Boruta tests both positive and negative hypothesis. Therefore, it is able to determine whether a feature is important, unimportant, or be undecided.

8.2.6 Ground-truth check

The synthetic dataset used in this section is described by the following causal graph:



where:

- Black variables are relevant for the target.
- Gray variables are latent.

- Red variables are irrelevant.

This graph has some common patterns:

Mediator A variable A that hides the effect of another variable B. If A affects the target, then B also does.

> **Example.** In the causal graph, X_2 is a mediator between X_0, X_1 and Y, which might cause problems to detect X_0 and X_1 as relevant features. X_2 also mediates for Z_0, which, in this case, has a positive effect as Z_0 is not observed.

> **Remark.** Strongly correlated features (e.g., mediator-mediator) might mislead algorithms when determining relevant features as a model might partition the importance between the two features.

Confounder A variable A that has effect on two variables B_1 and B_2. Therefore, it correlates B_1 and B_2. This might cause to mistakenly consider a variable important for predicting the target.

> **Example.** In the causal graph, Z_1 causes a confounder between X_0 and X_4. X_4 might be considered a relevant feature.

Overall, Boruta is able to:

- Identity all causal variables.
- Correctly estimate the distribution of almost all the variables.
- Determine monotonic effects and mediators.

9 Knowledge injection

Remark. ML models exploit implicit knowledge from the data. Explicit knowledge (e.g., rules-of-thumb, known correlations and causal factors, laws of physics, ...) is instead not used.

9.1 Approaches

9.1.1 Generative approach

Generative approach

Generative approach Use symbolic knowledge to create training samples that are used to train a model.

Remark. This approach does not let the model exploit explicit knowledge and might be inefficient.

9.1.2 Lagrangian approaches

Knowledge as constraint Use hard or soft constraints to inject knowledge.

Example (RUL estimation)**.** For RUL estimation, a simple explicit knowledge is that RUL decreases by 1 unit each time step. Formally, given two pairs of examples (x_i, y_i) and (x_j, y_j), it holds that:

$$y_i - y_j = j - i \quad \forall i, j = 1, \dots, m \text{ with } c_i = c_j$$

where c_k indicates the machine of the k-th sample. Given a model f, it can be constrained as follows:

$$f(x_i; \theta) - f(x_j; \theta) \approx j - i$$

Its training problem becomes:

$$\arg\min_{\theta} \mathcal{L}(y, f(x; \theta)) \text{ subj. to } f(x_i; \theta) - f(x_j; \theta) \approx j - i$$

Lagrangian approaches

Lagrangian approaches Given:

- A training problem: $\arg\min_\theta \{\mathcal{L}(\hat{y}) \mid \hat{y} = f(x; \theta)\}$,
- Some constraints defined as an inequality on a vector function $\mathbf{g}(\hat{y}) \leq 0$ with $\mathbf{g}(\hat{y}) = \{g_k(\hat{y})\}_{k=1}^m$.

Naive formulation The constraints can be formulated as a loss penalty as follows:

$$\mathcal{L}(\theta, \boldsymbol{\lambda}) = \mathcal{L}(\hat{y}) + \boldsymbol{\lambda}^T \mathbf{g}(\hat{y})$$

where $\boldsymbol{\lambda}$ is a vector of multipliers (Lagrangian multipliers).

Remark. $g_k(\hat{y}) = 0$ and $g_k(\hat{y}) \leq 0$ both satisfy the constraint. However, if $g_k(\hat{y})$ goes below 0, it becomes an unwanted reward.
In classical Lagrangian theory, this is solved by changing the sign of λ_k. However, this works by assuming convexity and requires optimizing for $\boldsymbol{\lambda}$.

Clipped formulation The constraints can be formulated as a loss penalty as follows:

$$\mathcal{L}(\theta, \boldsymbol{\lambda}) = \mathcal{L}(\hat{y}) + \boldsymbol{\lambda}^T \max\{0, \mathbf{g}(\hat{y})\}$$

with $\boldsymbol{\lambda} \geq 0$.

Remark. An equality constraint $g_k(\hat{y}) = 0$ can be formulated as:

$$g_k(\hat{y}) \leq 0 \wedge -g_k(\hat{y}) \leq 0$$

In penalty terms, it becomes:

$$\lambda'_k \max\{0, g_k(\hat{y})\} + \lambda''_k \max\{0, -g_k(\hat{y})\} = \lambda_k |g_k(\hat{y})|$$

where $\lambda_k = \lambda'_k + \lambda''_k$.
An alternative formulation is also:

$$\boldsymbol{\lambda}^T \mathbf{g}(\hat{y})^2$$

which is due to normal distribution properties.

Remark. Lagrangian approaches usually work with differentiable constraints, but it is not strictly required. However, differentiability is needed for training with gradient descent.

Multipliers calibration (maximal accuracy) Consider constraints in a soft manner. The penalty can be considered as a regularizer and $\boldsymbol{\lambda}$ can be considered as a hyperparameter and optimized through hyperparameter tuning.

Remark. This approach is viable when sufficient data is available.

Multipliers calibration (constraints satisfaction) Consider constraints in a hard manner.

Naive approach Use a large $\boldsymbol{\lambda}$.

Remark. This approach leads to numerical instability and disproportional gradients.

Dual ascent Dual ascent

Remark. The loss with the constraint penalty is differentiable in $\boldsymbol{\lambda}$:

$$\nabla_\lambda \mathcal{L}(\theta, \boldsymbol{\lambda}) = \max\{0, \mathbf{g}(f(x, \theta))\}$$

where:

- If the constraint is satisfied, the partial derivative is 0.
- If the constraint is violated, the partial derivative is equal to the violation.

Alternate gradient descent and ascent. The method works as follows:

1. Initialize the multipliers $\boldsymbol{\lambda}^{(0)} = 0$.
2. Until a stop condition is met:
   a) Obtain $\boldsymbol{\lambda}^{(k)}$ via gradient ascent with $\nabla_{\boldsymbol{\lambda}} \mathcal{L}(\theta^{(k-1)}, \boldsymbol{\lambda})$.
   b) Obtain $\theta^{(k)}$ via gradient descent with $\nabla_\theta \mathcal{L}(\theta, \boldsymbol{\lambda}^{(k)})$.

Remark. Lagrangian approaches are enforced at training time. Constraints might be violated at test time.

Example (RUL estimation)**.** The constraint:

$$f(x_i;\theta) - f(x_j;\theta) \approx j - i$$

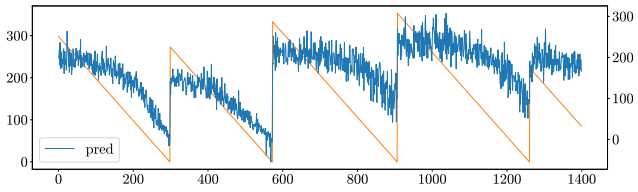
can be formulated as the following penalty:

$$\lambda \sum_{\substack{i,j=1,\dots,m \\ c_i=c_j}} (f(x_i;\theta) - f(x_j;\theta) - (j-i))^2$$

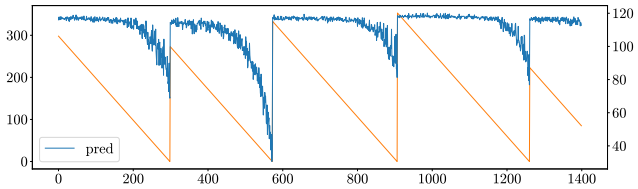
where λ is the same for all pairs for simplicity. Moreover, to avoid redundances, it is reasonable to only consider consecutive time steps (denoted as $i \prec j$):

$$\lambda \sum_{\substack{i \prec j \\ c_i=c_j}} (f(x_i;\theta) - f(x_j;\theta) - (j-i))^2$$

Remark. With batches, consecutivity refers to the closest available time step of the same machine in the same batch.
It is also necessary to sample batches in such a way that at least two time steps of the same machine are considered (otherwise the gradient step would be wasted).



(a) Results without knowledge injection



(b) Results with knowledge injection (note that the scales are off)

9.1.3 Ordinary differential equations learning

Ordinary differential equation (ODE) Equation defined as:

Ordinary differential equation (ODE)

$$\dot{y} = f(y,t)$$

where $\dot{y}$ is the rate of change and y is the state variable defined as a function of (usually) time t (i.e., $y(t)$ is the state at time t).

Remark. This class of differential equations can be seen as a transition system with continuous steps.

Remark. ODEs are useful to represent physics knowledge.

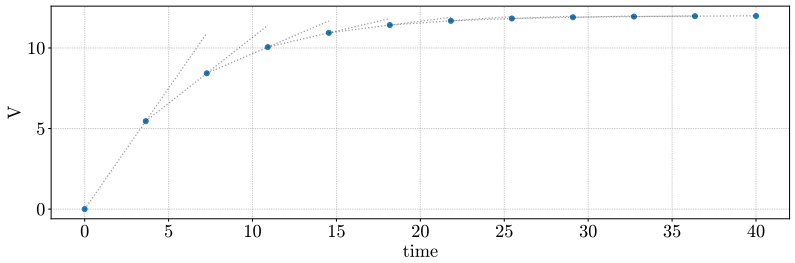
Initial value problem Given an ODE $\dot{y} = f(y,t)$ and an initial state $y(0) = y_0$, determine how the states unfold (i.e., run a simulation).

Initial value problem

Euler method Solve an initial value problem by discretizing time and computing the transition function at time t as: Euler method

$$y_k = y_{k-1} + (t_k - t_{k-1}) f(y_{k-1}, t_{k-1})$$

It is assumed that the solution is piece-wise linear (i.e., linearity between two consecutive states).



Remark. Euler method does not perform well in terms of accuracy. There are variants with better performance.

Learning ODE Estimate the parameters of an ODE from the data. The training problem is defined as: Learning ODE

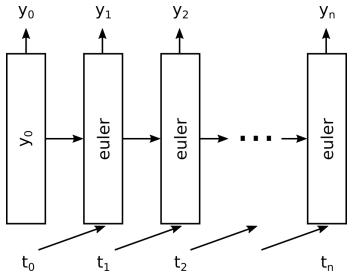
$$\arg\min_{\theta} \{\mathcal{L}(\hat{y}(t), y) \mid \dot{\hat{y}} = f(\hat{y}, t; \theta) \wedge \hat{y}(0) = y_0\}$$

A possible approach is to discretize time and optimize on the relaxed problem. The steps are:

1. Solve the initial value problem using a numerical method (e.g., Euler).
2. Compute the loss $\mathcal{L}$ and optimize over θ.

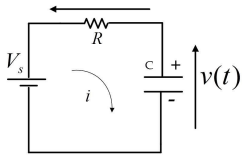
Remark. This path can be taken if the integration steps are differentiable. Euler method is differentiable.

Architecture The method can be implemented in an RNN fashion with the Euler method encoded into a repeated layer. At each step, the networks takes as input the state and the time variable, and estimates a new state.



Remark. This approach is slow to converge and is not very accurate.

Example. Consider an RC circuit with a voltage source V_S, a capacitor C, and a resistor R.



Its dynamic behavior is described by the ODE:

$$\dot{V} = \frac{1}{\tau}(V_S - V)$$

where $\tau = RC$.
Assume that we have a dataset of the ground-truth voltage y at each time step and we want to find the parameters V_S and τ of the ODE. The problem is defined as:

$$\arg\min_{V_S,\tau} \mathcal{L}(\hat{y}(t), y) \text{ subj. to } \dot{\hat{y}} = \frac{1}{\tau}(V_S - \hat{y}) \wedge \hat{y}(0) = y_0$$

A layer of the neural network estimates V_S and τ. The time steps are passed through the network and all the predicted voltages are used to compute the loss.
Note that V_S and τ must be positive values. We can use the same trick as in Section 7.2.1 by using exp log with a scaling factor to start with a reasonable guess.

ODE learning improvements

Training speed/Network depth Given a sequence of training measurements $\{y_k\}_{k=0}^n$, view them as a sequence of pairs $\{(y_{k-1}, y_k)\}_{k=1}^n$. During training, each pair trains a distinct ODE, each with shared parameters. The overall problem becomes:

$$\begin{aligned} &\arg\min_{\theta} \sum_{k=1}^{n} \mathcal{L}(\hat{y}_k(t_k), y_k) \\ \text{subject to } &\dot{\hat{y}}_k = f(\hat{y}_k, t; \theta) \qquad \forall k = 1, \ldots, n \\ &\hat{y}_k(t_{k-1}) = y_{k-1} \qquad \forall k = 1, \ldots, n \end{aligned}$$

Remark. This approach is only possible if full states are available and the loss is separable. Moreover, it is not strictly equivalent to the original problem as compound errors are disregarded.

Remark. Training now requires shallower networks and mini-batches can be used.

Accuracy improvement Accuracy issues are due to the fact that the Euler method intrinsically has low performance. As the problem consists of fitting a curve, the model might need to estimate wrong parameters to achieve a better result.

Therefore, if the objective is to fit a curve, this is not necessarily a problem. However, if the correct parameters are the goal, a more accurate integration method is needed.

Remark. A straightforward approach to achieve better results is to increase the granularity of the steps of the Euler method (i.e., use more steps).

Universal ODE (UDE) Use black-box functions as the parameter of an ODE:

Universal ODE (UDE)

$$\dot{y} = f(y, t, U(y, t; \theta))$$

where U is a universal approximator (e.g., a neural network).

Example. Consider the SIR (susceptible-infected-recovered) model for epidemic

modeling:

$$\begin{aligned}\dot{S} &= -\beta\frac{1}{N}SI \\ \dot{I} &= +\beta\frac{1}{N}SI - \gamma I \\ \dot{R} &= +\gamma I\end{aligned}$$

Non-pharmaceutical interventions (NPI) (e.g., masks) have an effect on β, making it time dependent:

$$\begin{aligned}\dot{S} &= -\beta(t)\frac{1}{N}SI \\ \dot{I} &= +\beta(t)\frac{1}{N}SI - \gamma I \\ \dot{R} &= +\gamma I\end{aligned}$$

For this example, we assume $\beta(t)$ is modeled as:

$$\beta(t) = \beta_0 \prod_{i \in \mathcal{I}} e_i$$

where β_0 is the baseline spread if nothing is done, $\mathcal{I}$ is the set of active NPIs, and e_i is the effect of the i-th NPI.
In practice, the time argument for β is to retrieve the active NPIs at time t, therefore, the overall model can be formulated as:

$$\begin{aligned}\dot{S} &= -\beta(\texttt{NPI}(t))\frac{1}{N}SI \\ \dot{I} &= +\beta(\texttt{NPI}(t))\frac{1}{N}SI - \gamma I \\ \dot{R} &= +\gamma I\end{aligned}$$

Architecturally, a neural network as in ODE can be used. The only addition is that it takes as input the active NPIs.

9.1.4 Physics informed neural network

Physics informed neural network (PINN) Use a neural network to predict the state at time t:

Physics informed neural network (PINN)

$$\hat{y}(t;\theta) \approx y(t)$$

Remark. ODEs predict the derivative of the change of the state, while PINNs directly predict the next state. This allows for faster inference as integration (i.e., Euler method) is no longer needed.

Training The training objective is similar to the one of UDE, with some changes to the constraints:

$$\begin{gathered}\arg\min_{\theta} \mathcal{L}(\hat{y}(t,\theta), y) \\ \text{subject to } \dot{\hat{y}}(t;\theta) = f(\hat{y}(t;\theta), t) \\ \hat{y}(t_0;\theta) = y_0\end{gathered}$$

where the first constraint imposes some physics knowledge and depends on the input (not the parameters).

Remark. A PINN can be seen as neural network that learns ODE integration.

In practice, the overall loss can be formulated as a Lagrangian:

$$\begin{aligned}\mathcal{L}(y, \hat{y}, t, \theta) =& \mathcal{L}(\hat{y}(t;\theta), y) \\ &+ \lambda_{de}^T \|\dot{\hat{y}}(t;\theta) - f(\hat{y}(t;\theta), t)\|_2^2 \\ &+ \lambda_{bc}^T \|\dot{\hat{y}}(t;\theta) - y_0\|_2^2\end{aligned}$$

where λ_{de}^T and λ_{bc}^T are multipliers.

Remark. If needed, the loss can be generalized further.

Remark. If the physics (f) is known, the two constraints can be enforced without data points as only time steps (which can be discretized and decided a priori) are needed. Moreover, the derivative ($\dot{\hat{y}}(t;\theta)$) w.r.t. t can be computed using automatic differentiation.
Therefore, during training, it is possible to rely on the two constraints more than the loss.

Remark. Finding the weights λ_{de}^T and λ_{bc}^T can be tricky depending on the reliability and robustness of the physics model that is used. Cross-validation can be used if unsure and dual ascent can be used if the model is trusted.

10 Predict and optimize

10.1 Approaches

10.1.1 Prediction focused learning

Prediction focused learning

Prediction focused learning Inference method that solves an optimization problem by using inputs predicted by an estimator. More specifically, there are two steps:

Predict Train a predictor for the parameters of the problem. The optimal predictor h has the following parameters:

$$\theta^* = \arg\min_{\theta} \left\{ \mathbb{E}_{(x,y)\sim P(X,Y)}[\mathcal{L}(y, \hat{y})] \mid \hat{y} = h(x, \theta) \right\}$$

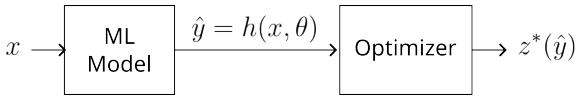
Optimize Solve an optimization problem with the estimated parameters as input:

$$z^*(y) = \arg\min_{\mathbf{z}} \{ f(\mathbf{z}, y) \mid \mathbf{z} \in F \}$$

where $\mathbf{z}$ is the decision vector, f is the cost function, F is the feasible space, and y is the output of the predictor h.

Therefore, during inference, the following is computed:

$$z^*(h(x; \theta)) = z^*(\hat{y})$$



Remark. This approach is asymptotically correct. The perfect predictor allows to reach the optimal result.

Remark. The predictor should be trained for minimal decision cost (instead of maximal accuracy) so that the optimizer can make the correct choice.

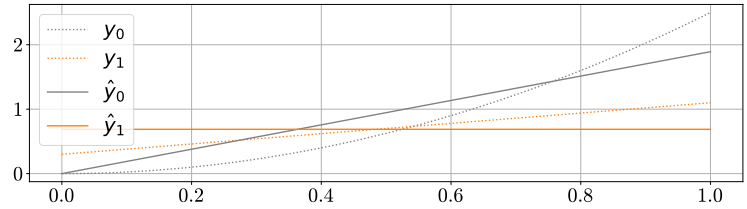
Example. Consider the problem:

$$\arg\min_{z} \{ y_0 z_0 + y_1 z_1 \mid z_0 + z_1 = 1, z \in \{0, 1\}^2 \}$$

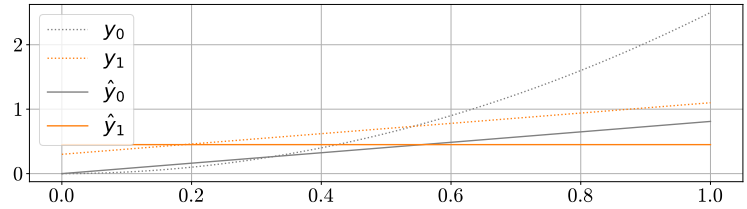
with some ground-truth y_0 and y_1. Assume that the predictor can only learn a model of form:

$$\hat{y}_0 = \theta^2 x \qquad \hat{y}_1 = 0.5 \cdot \theta$$

By maximizing accuracy, the following predictions are obtained:



The intersection point is important for optimization. In this case, predictions are not ideal. Instead, by minimizing decision cost, the following predictions are made:



10.1.2 Decision focused learning

Decision focused learning (DFL) PFD where linear cost functions are assumed. The optimization problem is therefore: Decision focused learning (DFL)

$$z^*(y) = \arg\min_z \{y^T z \mid z \in F\}$$

where y cannot be measured but depends on some observable x (i.e., $X, Y \sim P(X, Y)$).

The training problem of the predictor aims to minimize the decision cost and is defined as:

$$\theta^* = \arg\min_\theta = \left\{\mathbb{E}_{(x,y)\sim P(X,Y)} \left[\texttt{regret}(y, \hat{y}) \mid \hat{y} = h(x, \theta)\right]\right\}$$

Regret Measures the difference between the solution obtained using the predictor and the perfect solution. It is defined as: Regret

$$\texttt{regret}(y, \hat{y}) = y^T z^*(\hat{y}) - y^T z^*(y)$$

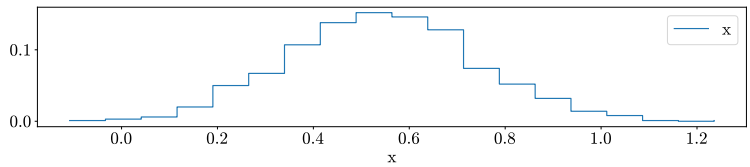
where:

- $z^*(y)$ is the best solution with access to the ground-truth (i.e., an oracle).
- $z^*(\hat{y})$ is the solution computed with the estimated parameters.

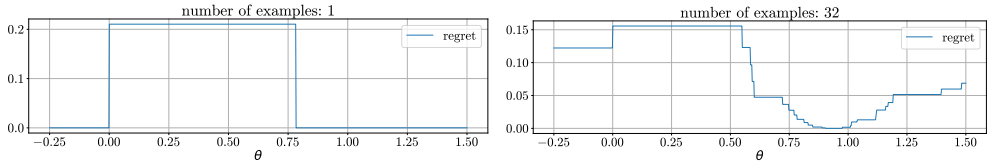
Remark. Optimizing regret is equivalent to optimizing the cost function, but regret is lower-bounded at 0.

Remark. Regret is non-differentiable in many points and, when it is, its gradient is not informative. In practice, a surrogate for regret is used instead.

Example. Consider a collection of normally distributed data (x, y):



The regret landscape for varying parameter θ is:



(a) Regret for a single sample (b) Regret for a batch

Self-contrastive loss Surrogate for regret defined as: Self-contrastive loss

$$\hat{y}^T z^*(y) - \hat{y}^T z^*(\hat{y})$$

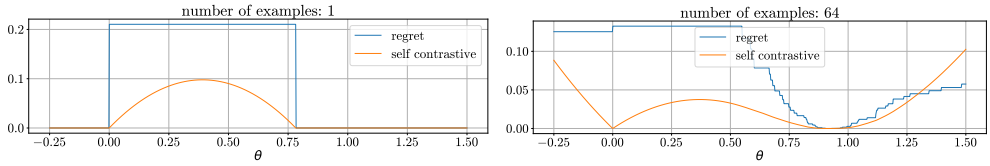
The idea is that a good prediction vector $\hat{y}$ should make the optimal cost $\hat{y}^T z^*(y)$ not worse than the cost of the estimated one $\hat{y}^T z^*(\hat{y})$.

Remark. By differentiating over $\hat{y}$, the result is a subgradient (i.e., coefficient used to compute a non-defined gradient) and it is computed as:

$$\nabla(\hat{y}^T z^*(y) - \hat{y}^T z^*(\hat{y})) = z^*(y) - z^*(\hat{y})$$

Remark. Self-contrastive loss creates spurious minima (i.e., false minima that are not in the regret) as a trivial solution is to predict $\hat{y} = 0$.

Example. The self-contrastive loss using the same data as before is:



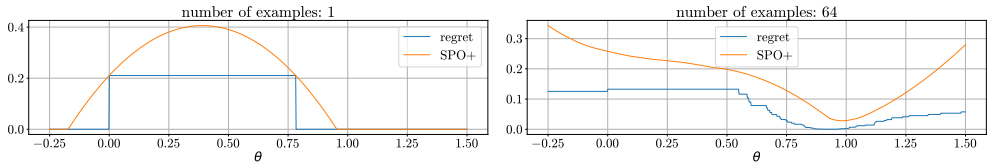
(a) Self-contrastive loss for a single sample (b) Self-contrastive loss for a batch

SPO+ loss Surrogate for regret defined as a perturbed version of the self-contrastive loss: SPO+ loss

$$\texttt{spo+}(y, \hat{y}) = \hat{y}_{\text{spo}}^T z^*(y) - \hat{y}_{\text{spo}}^T z^*(\hat{y}_{\text{spo}}) \qquad \text{with } \hat{y}_{\text{spo}} = 2\hat{y} - y$$

Remark. With many samples, the spurious minima tend to cancel out.

Example. The SPO+ loss using the same data as before is:



(a) SPO+ for a single sample (b) SPO+ for a batch

Remark. DLF are slow to train as each iteration requires to solve an optimization problem.

DLF training speed-up

Warm start Initialize a DFL network with PFL weights.

Solution caching Assuming that the feasible space is constant, caching can be done as follows:

1. Initialize the cache $\mathcal{S}$ with the true optimal solutions $z^*(y_i)$.

2. When it is required to compute $z^*(\hat{y})$:
   - With probability p, invoke the solver and compute the real solution. The newly computed value is cached.
   - With probability $p - 1$, do a cache lookup as:

$$\hat{z}^*(\hat{y}) = \arg\min_z \{f(z) \mid z \in \mathcal{S}\}$$

Remark. PFL with more complex networks allows reaching comparable performance to DLF.