AIHack2020

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March 1, 2020

Code

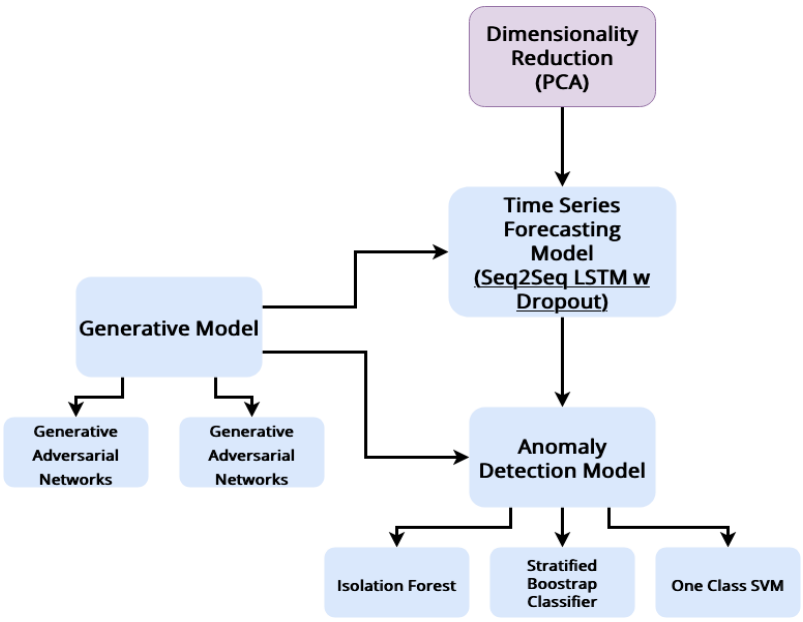
A notebook containing our code/visualisations is available here and our Github repo is available here

Motivation and Solution

The aim our solution is to create a pipeline of models that can "understand" the data generating process (using GANs or Autoencoders), produce a probabilistic forecast of future measurements (Forecasting using Seq2Seq LSTM with Dropout) , and at each step produce a probability of an anomaly (An ensemble of anomaly detection methods).

By being able to understand latent structure of the data and what conditions that are more likely to be associated with *anomalies* advance planning can be done, leading to significant reductions in maintenance costs and time, and also increasing work safety.

This solution would take the form of a dashboard built in Flask and Plotly, in which the user can generate synthetic data and a corresponding forecast. Given the time constraints, we were not able to complete this, but have made progress on the underlying models.



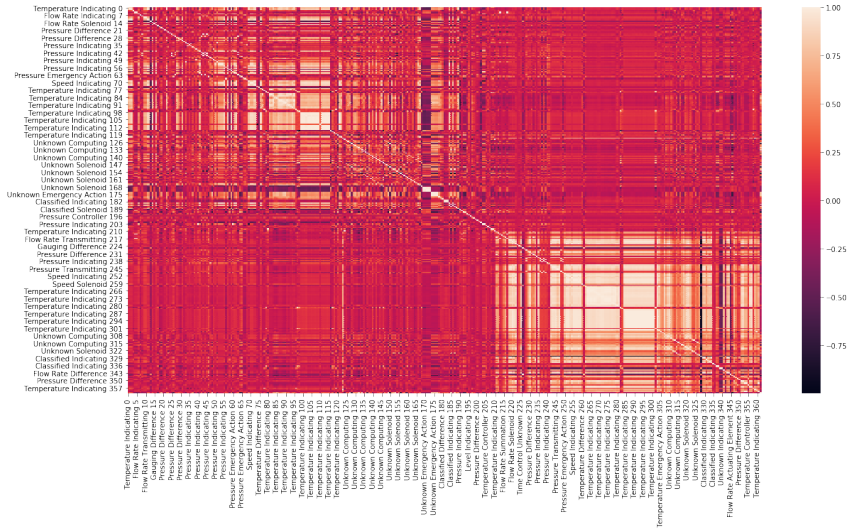
Data Description

We are given a preprocessed dataset *clean_data.csv*, consisting of 106710 observations with 362 features, corresponding to sensor readings for a single *asset*, a "low pressure compressor". 9 indices corresponding to 9 automatic overrides were also provided, associated with the raw dataset *raw_data.csv*

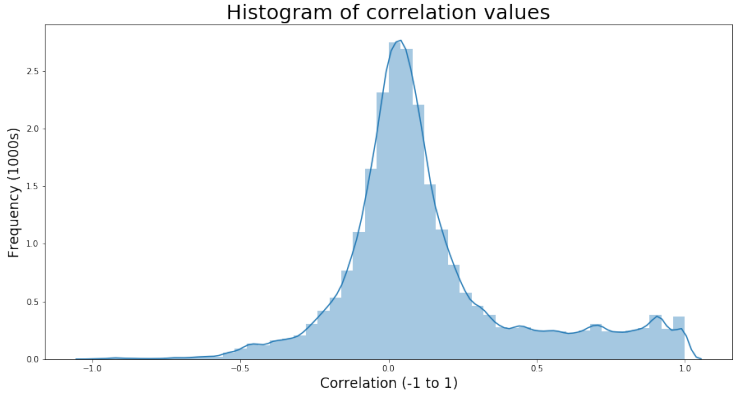
The Preprocessing that has been done for us: datapoints for which "Temperature too low (below 80)" and "Exit pressure too high (above 58)" are removed without smoothing, and features with more than 4 hours missing continuous data, more than 5% total data missing are dropped.

Data Exploration

The data is too high in dimensionality for individual plots; we plot a correlation matrix and observe that there is significant correlation for certain features.



A histogram of correlation values shows that this is indeed this is the case; The distribution of correlations roughly follows a normal with $\mu = 0.1347$, $\sigma = 0.3067$ bounded in $[-1, 1]$

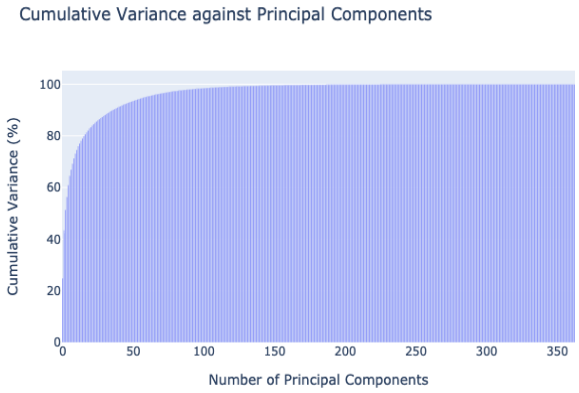


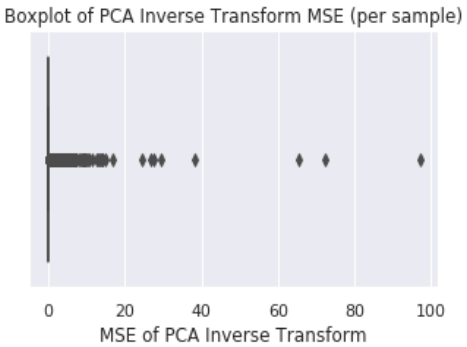
Dimensionality Reduction

The high dimensionality of the data, coupled with the correlation between features suggested that dimensionality reduction was a good first step, in order to both reduce complexity for use in further models, and also for feature extraction/ to model a latent space. We attempted two principal approaches: Principal Components Analysis and Autoencoders.

Principal Components Analysis

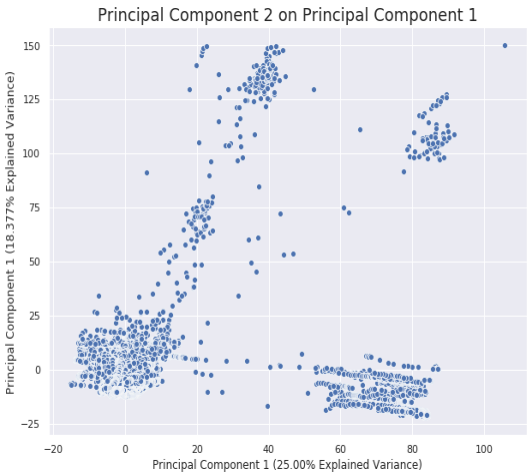
We first experimented with dimensionality reduction using PCA in sklearn. The data is standardised using sklearn's StandardScaler, with missing values zero-filled; this makes the assumption that each feature is Gaussian and Stationary, which may not necessarily be correct. Feature imputation methods could also be considered as a next step but is costly in terms of time.

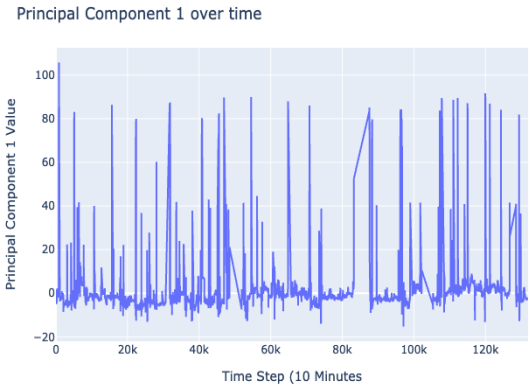




80% and 90% of the explained variance is given by the top 16 and 36 principal components, respectively. With 36 principal components, the mean MSE of an inverse transform (assuming all features are equally important) is 0.101288 with 0.5% of samples exceeding a MSE of 1. These 'outliers' could be potentially be further utilised in the anomaly detection.

We can visualise the latent structure of the data:





Other Dimensionality Reduction

We also attempted but discarded approaches using Kernel PCA, due to its high time complexity, and Agglomerate Clustering, as without more explicit engineering it would be limited to merging the features linearly.

Autoencoders

We compare PCA with dimensionality reduction with Autoencoders. We stack fully connected Dense Relu Layers

Generative Models

The purpose of generative models, in this context is to create "realistic" synthetic data that can be used for stress testing; if Shell can simulate measurements of the compressor, they can evaluate potential business/financial impacts and preemptively plan.

Variational Autoencoders

We can adapt the autoencoder to generate samples. The next step would be incorporate LSTM layers to consider the temporal structure.

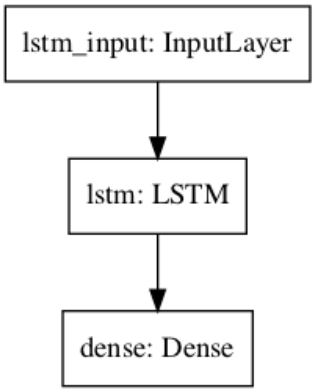
Generative Adversarial Networks

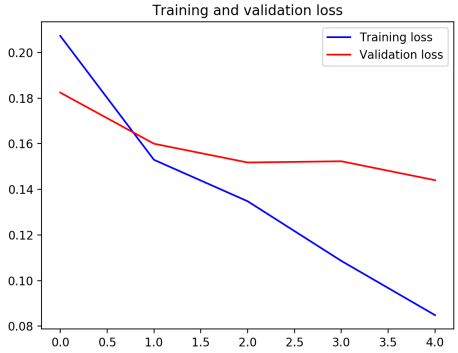
We had no time to implement this, but it would be another approach to generating "realistic" synthetic data.

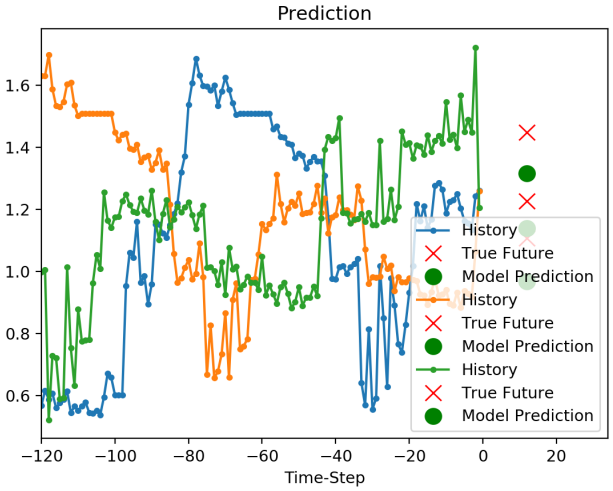
Time Series Forecasting

We began by considering forecasting for individual features using Gaussian Process Regression and ARIMA. The constraints of the former are its intense memory usage (at least its sklearn implementation) and asserting that the distribution through time is Gaussian, and the latter in its inability to capture non-linearities.

We then proposed to implement a Sequence-to-Sequence LSTM as a way to forecast the $T + K$ measurements (next $10K$ minutes) using a window W of $T - W$ past observations. We were limited by the processing abilities of Colab and time allocated.







A next step would be to make it Bayesian; incorporate Dropout layers as a way of generating probabilistic predictions confidence intervals.

Anomaly Detection

With only 9 indices known to correspond to anomalies (automatic overrides), our initial intention was to use unsupervised outlier detection methods to identify any other potential anomalies and take an *ensemble*:

Isolation Forest

We fit a Isolation Forest to the standardised *clean_data.csv*, which we shall term X, with the following parameters: **100 estimators, subsampling 70% of features, with bootstrap**. The model detects 3351 outliers, or 3.14% of the data

The advantage of Isolation Forests are that it can learn non-linear structures and multi-modalities, the disadvantages is that this method is not interpretable.

One Class SVM

We fit a linear One Class SVM, first on the standardised data X, and then on the PCA transformed data X_{pca}. This makes the assumption that anomalies are linearly seperable.

The advantage of this is that it is interpretable (given its linear decision boundary), but the running time (O(n^3) takes too long to render it practical.

Imbalanced Classification

Given the relative limitations of the two unsupervised methods, we discarded the previous methods and experimented with treating the problem as an imbalanced classification problem.
We use a stratified bootstrap method; we undersample non-anomalies and keep all anomalies and concatenate them into training set df_i with target variable y (whether it is an anomaly).

For each df_i, we fit a classifier $f_i : df_i \rightarrow y_i$. We require a classifier that can return probabilistic estimates such as Logistic Regression (sklearn), Gradient Boosted Decision Tree (CatBoost), or Bayesian Networks. We repeat this for $N = 100$ rounds, and take the average of the feature importances $I \in R^{|F|}$. $\hat{I} = \frac{1}{N} \sum I$, . For Logistic Regression this could be the magnitude of coefficients, CatBoost the in built feature importance and Bayesian Networks Shapley Values. This allows us to determine the association between each feature and an anomaly occurring. We can further take an ensemble of these classifiers.

In this case we undersampled non-anomalies, another avenue to explore could be to use SMOTE to oversample anomalies.

Further Development

Our models (apart from the time series forecasting) in general, i.e. those for dimensionality reduction and anomaly detection have made little use of the temporal structure of the data; this could be an avenue to be further explored in the future, however in the context of AIHack we were heavily constrained by time and our lack of knowledge

Bibliography

1.

2.

3.

Is this a hot dog or not a hot dog?