Autoencoders for Anomaly Detection

High Performance Computing

HPC refers to HW/SW infrastructures for particularly intensive workloads

High Performance Computing

HPC is (somewhat) distinct from cloud computing

- Cloud computing is mostly about running (and scaling services)
- ...HPC is all about performance

Typical applications: simulation, massive data analysis, training large ML models

HPC systems follow a batch computation paradigm

- Users send jobs to the systems (i.e. configuration for running a program)
- Jobs end in one of several queues
- A job scheduler draws from the queue
- ...And dispatches jobs to computational nodes for execution

High Performance Computing

HPC systems can be large and complex

E.g. Leonardo, the 4-th most powerful supercompuer (as of June 2023)

4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404

- The system has 1,824,768 cores overall!

Configuring (and maintaining the configuration) of these systems

- ...Is of very important, as it has an impact on the performance
- ...And very challenging, due to their scale and the to node heterogeneity

Hence the interest in detecting anomalous conditions

The Dataset

As an example, we will consider the DAVIDE system

Small scale, energy-aware architecture:

- Top of the line components (at the time), liquid cooled
- An advanced monitoring and control infrastructure (ExaMon)
- ...Developed together with UniBo

The system went out of production in January 2020

The monitoring system enables anomaly detection

- Data is collected from a number of samples with high-frequency
- Long term storage only for averages over 5 minute intervals
- Anomalies correspond to unwanted configurations of the frequency governor
- ...Which can throttle performance to save power or prevent overheating

A Look at the Dataset

Our dataset refers to the non-idle periods of a single node

In [8]:
```python
print(f'#examples: {hpc.shape[0]}, #columns: {hpc.shape[1]}')
hpc.iloc[:3]
```

```
#examples: 6667, #columns: 161
```

Out[8]:

	timestamp	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12	cmbw_p0_13	cmbw_p0_14	cmbw_p0_2
0	2018-03-05 22:45:00	0.165639	0.006408	0.012176	0.166835	0.238444	0.230092	0.145691	0.227682	0.000094
1	2018-03-05 22:50:00	0.139291	0.007772	0.057400	0.166863	0.238485	0.230092	0.145691	0.227682	0.176855
2	2018-03-05 22:55:00	0.141048	0.000097	0.000000	0.166863	0.238444	0.230092	0.145691	0.227682	0.252403

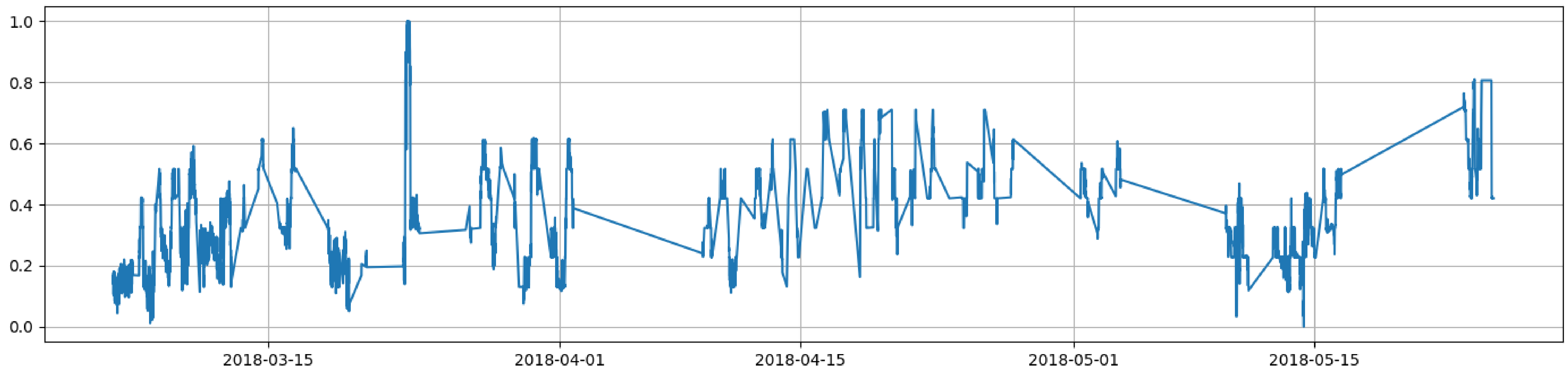
3 rows × 161 columns

- This still a time series, but a multivariate one

A Look at the Dataset

How to display a multivariate series? Approach #1: showing individual columns

```
In [12]: tmp = pd.Series(index=hpc['timestamp'], data=hpc[inputs[0]].values)
         util.plot_series(tmp, figsize=figsize)
```



- The series contains significant gaps (i.e. the idle periods)

A Look at the Dataset

Approach #2: obtaining statistics

In [13]:
```
hpc[inputs].describe()
```

Out[13]:

	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12	cmbw_p0_13	cmbw_p0_14	cmbw_p0_2
count	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000	6667.000000
mean	0.357036	0.138162	0.060203	0.119616	0.160606	0.184970	0.118305	0.151434	0.143033
std	0.166171	0.128474	0.090796	0.098597	0.128127	0.163190	0.104490	0.120793	0.125052
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.227119	0.000073	0.000020	0.000000	0.000000	0.000000	0.000000	0.000000	0.000117
50%	0.323729	0.136095	0.000082	0.166835	0.238444	0.230092	0.145691	0.227682	0.174933
75%	0.470254	0.261908	0.134976	0.166984	0.238566	0.230406	0.145908	0.227779	0.251910
max	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000

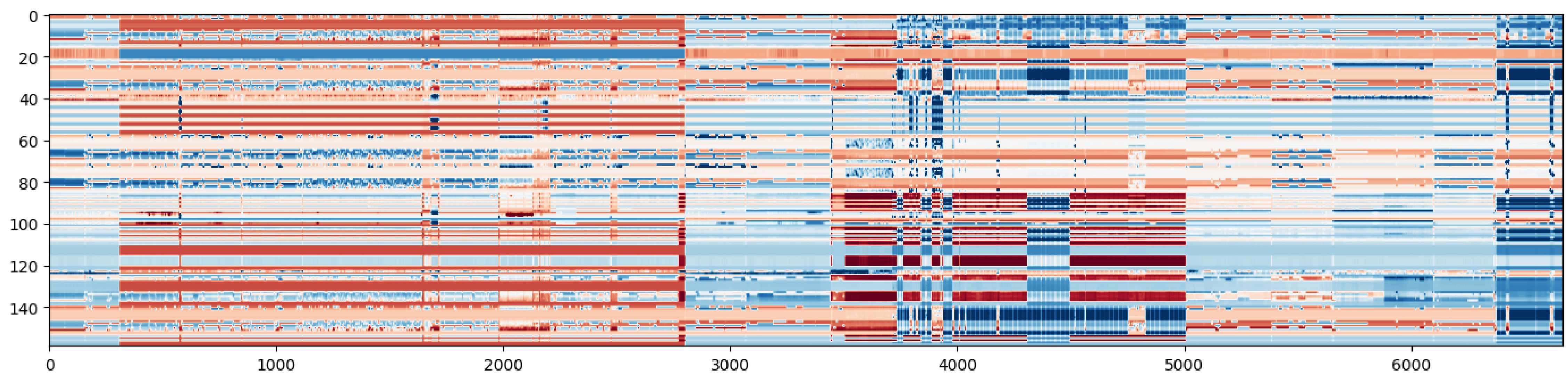
8 rows × 159 columns

- No missing value, normalized data

A Look at the Dataset

Approach #3: standardize, then use a heatmap

In [16]:
```
hpcsv = hpc.copy()
hpcsv[inputs] = (hpcsv[inputs] - hpcsv[inputs].mean()) / hpcsv[inputs].std()
util.plot_df_heatmap(hpcsv[inputs], figsize=figsize)
```



- White = mean, red = below mean, blue = above mean

Anomalies

There are three possible configurations of the frequency governor:

- Mode 0 or "normal": frequency proportional to the workload
- Mode 1 or "power saving": frequency always at the minimum value
- Mode 2 or "performance": frequency always at the maximum value

On this dataset, this information is known

...And it will serve as our ground truth

- We will focus on discriminating normal from non-normal behavior
- I.e. we will treat both "power saving" and "performance" configurations as anomalous

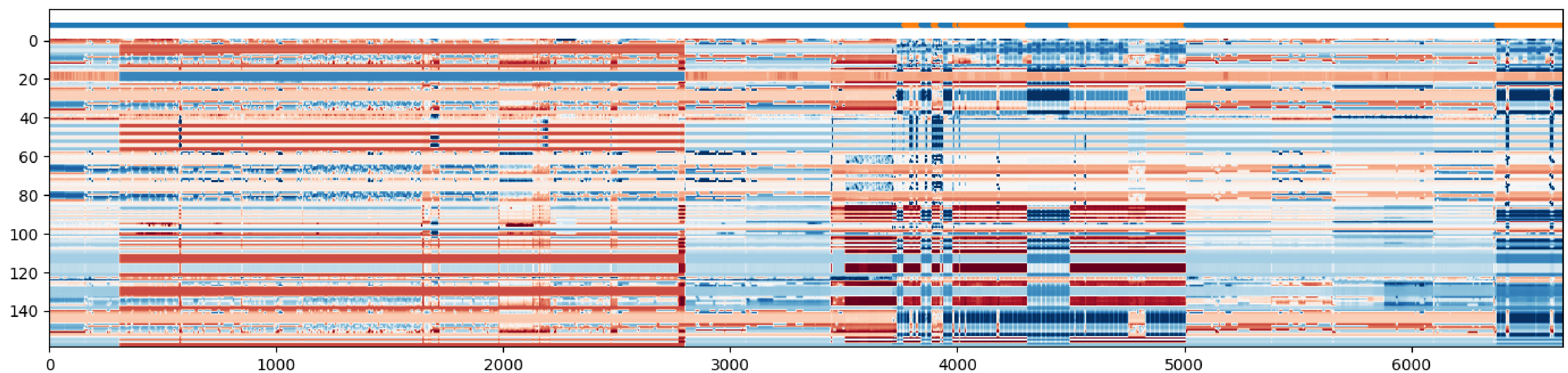
Detecting them will be challenging

- Since the signals vary so much when the running job changes

Anomalies

We can plot the location of the anomalies:

In [20]:
```
labels = pd.Series(index=hpcsv.index, data=(hpcsv['anomaly'] != 0), dtype=int)
util.plot_df_heatmap(hpcsv[inputs], labels, figsize=figsize)
```



- On the top, blue = normal, orange = anomaly

Autoencoders for Anomaly Detection

Autoencoders

An autoencoder is a type of neural network

The network is designed to reconstruct its input vector

- The input is some tensor x and the output should be the same tensor x

Autoencoders can be broken down in two halves

- An encoding part, i.e. $encode(x, \theta_e)$, mapping x into a vector of latent variables z
- A decoding part, i.e. $decode(z, \theta_d)$, mapping z into reconstructed input tensor

Autoencoders are trained so as to satisfy:

$$decode(encode(\hat{x}_i, \theta_e), \theta_d) \simeq \hat{x}_i$$

- I.e. $decode$, when applied to the output of $encode$
- ...Should approximately return the input vector itself

A nice introduction and tutorial about autoencoders can be found on the Keras

Autoencoders

Formally, we typically employ an MSE loss

$$L(\theta_e, \theta_d) = \sum_{i=1}^{n} \|\hat{x}_i - decode(encode(\hat{x}_i, \theta_e), \theta_d)\|_2^2$$

- This is trivial to satisfy if both $encode$ and $decode$ learn an identity relation
- ...So we need to prevent that

There are two main approaches to avoid learning a trivial mapping

- Using an information bottleneck, i.e. making sure that z has fewer dimensions that x
- Use a regularization to enforce sparse encodings, e.g.:

$$L(\theta_e, \theta_d) = \sum_{i=1}^{n} \|\hat{x}_i - decode(encode(\hat{x}_i, \theta_e), \theta_d)\|_2^2 + \alpha \|encode(x, \theta_e)\|_1$$

Autoencoders for Anomaly Detection

Autoencoders can be used for anomaly detection

...By using the reconstruction error as an anomaly signal, e.g.:

$$\| x - decode(encode(x, \theta_e), \theta_d) \|_2^2 > \theta$$

This approach has some PROs and CONs:

- Compared to KDE
  - Neural Networks have good support for high dimensional data
  - ...Plus limited overfitting and fast prediction/detection time
  - However, error reconstruction can be harder than density estimation
- Compared to autoregressors
  - Reconstructing an input is easier than predicting the future
  - ...So, we tend to get higher reliability

Autoencoders in Keras

Let's build an autoencoder in practice (with tensorflow 2.0 and keras)

First, we build the model

```
In [58]: input_shape = (len(inputs), )
         ae_x = keras.Input(shape=input_shape, dtype='float32')
         ae_z = layers.Dense(64, activation='relu')(ae_x)
         ae_y = layers.Dense(len(inputs), activation='linear')(ae_z)
         ae = keras.Model(ae_x, ae_y)
```

In this case, we used the keras functional API

- `Input` builds the entry point for the input data
- `Dense` builds a fully connected layer
- "Calling" layer A with parameter B attaches B to A
- `Model` builds a model object with the specified input and output

Autoencoders in Keras

Then we compile (prepare for training) the model

In [59]:
```
ae.compile(optimizer='adam', loss='mse')
```

Finally we can start training:

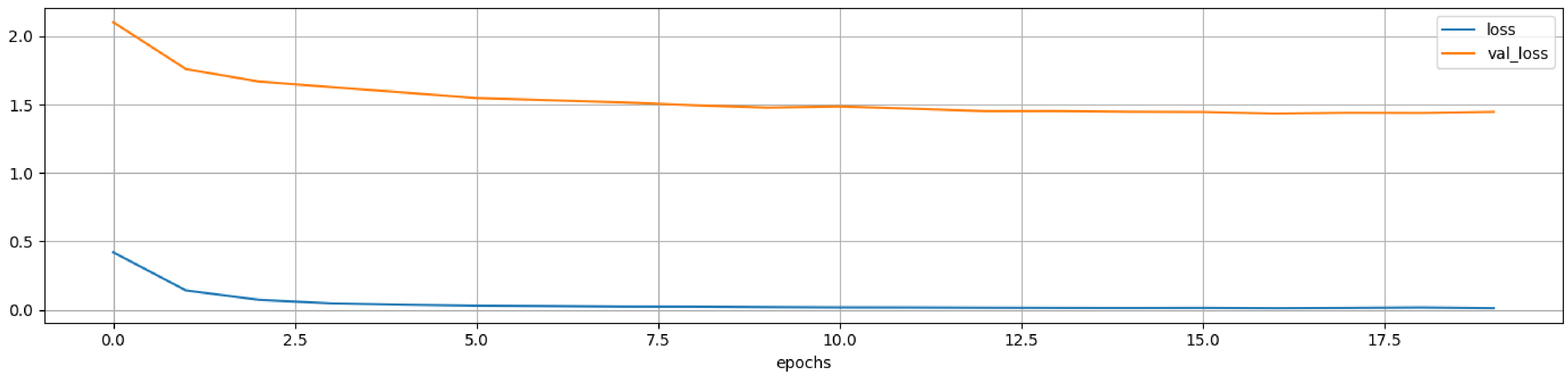
In [60]:
```
cb = [callbacks.EarlyStopping(patience=3, restore_best_weights=True)]
history = ae.fit(trdata[inputs], trdata[inputs], validation_split=0.1,
                 callbacks=cb,
                 batch_size=32, epochs=20, verbose=0)
```

- We are using a callback to stop training early
- ...If no improvement on the validation set is observed for 3 epochs

Autoencoders in Keras

Let's have a look at the loss evolution over different epochs

In [61]:
```
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.0115 (training), 1.4466 (validation)
```

Autoencoders in Keras

Finally, we can obtain the predictions

In [62]:
```
preds = pd.DataFrame(index=hpcs.index, columns=inputs, data=ae.predict(hpcs[inputs], verbose=0))
preds.head()
```

Out[62]:

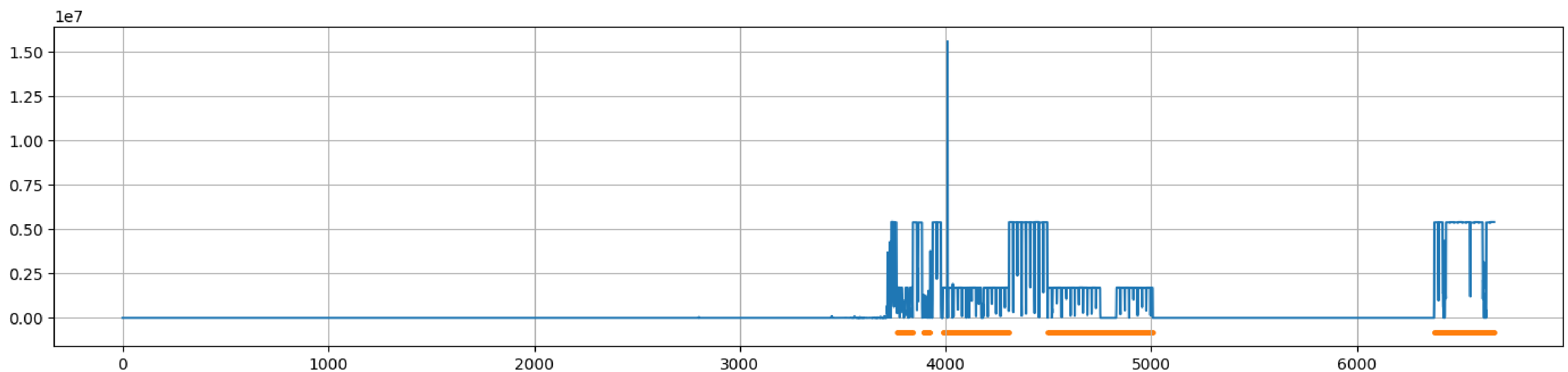
	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12	cmbw_p0_13	cmbw_p0_14	cmbw_p0_2	cmbw_p0_3
0	-1.979992	-0.437968	-0.524496	2.281610	2.480476	1.467216	1.875573	2.428959	-2.048617	-1.358454
1	-1.140026	-0.588035	-0.124288	2.012357	2.226431	2.237622	2.147029	1.925013	0.634144	-1.050098
2	-1.076701	-0.812375	-0.401593	2.441159	2.250029	2.344752	2.190624	2.400508	0.405078	0.488687
3	-1.223841	-0.726853	-0.606458	2.049987	2.119531	2.416896	2.235084	2.144840	0.835476	0.716049
4	-1.258236	-0.743420	-0.493074	2.221673	2.265017	2.282504	2.310348	2.232695	0.925034	0.711455

5 rows × 159 columns

Alarm Signal

We can finally obtain our alarm signal, i.e. the sum of squared errors

In [63]:
```
sse = np.sum(np.square(preds - hpcs[inputs]), axis=1)
signal_ae = pd.Series(index=hpcs.index, data=sse)
util.plot_signal(signal_ae, labels, figsize=figsize)
```



- It is actually quite similar to the KDE signal

Threshold Optimization

Then we can optimize the threshold as usual

In [64]:
```python
th_range = np.linspace(5e5, 1e6, 100)
th_ae, val_cost_ae = util.opt_threshold(signal_ae[tr_end:val_end],
                                        hpcs['anomaly'][tr_end:val_end],
                                        th_range, cmodel)
print(f'Best threshold: {th_ae:.3f}')
tr_cost_ae = cmodel.cost(signal_ae[:tr_end], hpcs['anomaly'][:tr_end], th_ae)
print(f'Cost on the training set: {tr_cost_ae}')
print(f'Cost on the validation set: {val_cost_ae}')
ts_cost_ae = cmodel.cost(signal_ae[val_end:], hpcs['anomaly'][val_end:], th_ae)
print(f'Cost on the test set: {ts_cost_ae}')
```

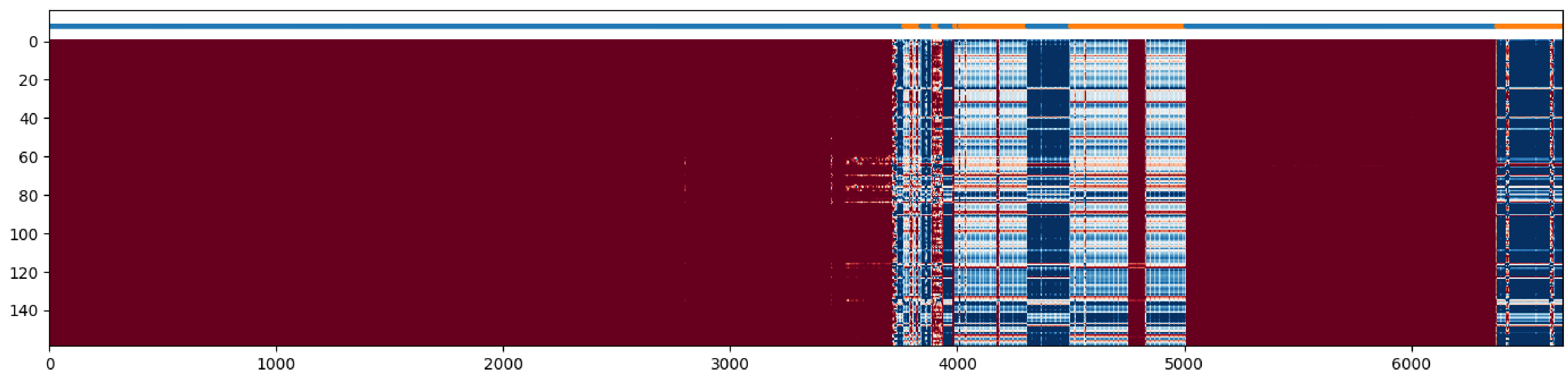
```
Best threshold: 939393.939
Cost on the training set: 0
Cost on the validation set: 248
Cost on the test set: 275
```

Mutiple Signal Analysis

But autoencoders do more than just anomaly detection!

- Instead of having a single signal we have many
- So we can look at the individual reconstruction errors

In [65]:
```
se = np.sqrt(np.square(preds - hpcs[inputs]))
signals_ae = pd.DataFrame(index=hpcs.index, columns=inputs, data=se)
util.plot_df_heatmap(signals_ae, labels, vmin=np.quantile(se, 0.25), vmax=np.quantile(se, 0.75),
```

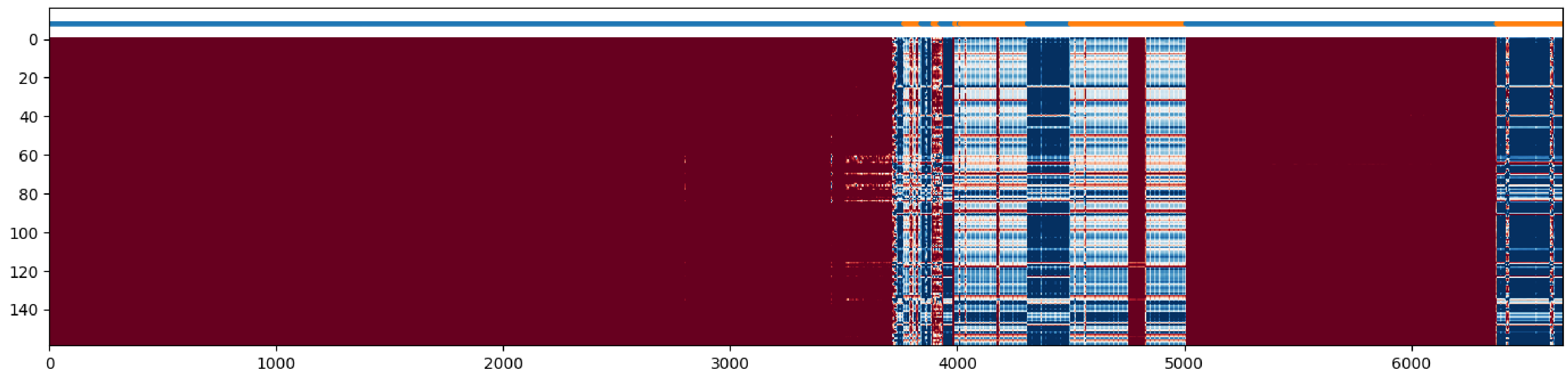


Mutiple Signal Analysis

Reconstruction errors are often concentrated on a few signals

- These correspond to the properties of the input vector that were harder to reconstruct
- ...And often they are useful clues about the nature of the anomaly

In [67]:
```
se = np.sqrt(np.square(preds - hpcs[inputs]))
signals_ae = pd.DataFrame(index=hpcs.index, columns=inputs, data=se)
util.plot_df_heatmap(signals_ae, labels, vmin=np.quantile(se, 0.25), vmax=np.quantile(se, 0.75),
```



Multiple Signal Analysis

Let's focus on the last mode 1 anomaly ("power saving" mode)

Here are the 8 largest errors in descending order

```
In [68]: last_mode_1 = hpcs.index[hpcs['anomaly']==1][-1]
         se.iloc[last_mode_1].sort_values(ascending=False)[:8]

Out[68]: ips_p0_14      549.640137
         ips_p0_10      467.667583
         ips_p0_12      461.034925
         ips_p0_11      360.061199
         ips_p0_8       277.142111
         ips_p0_9       189.797284
         util_p0_8      172.477909
         util_p0_11     169.846732
         Name: 5006, dtype: float64
```

- They are mostly related to performance (e.g. "ips" - Instructions Per Second)
- ...As it should be!

Multiple Signal Analysis

Now, let's move to the last mode 2 anomaly ("performance" mode)

Here are the 8 largest errors in descending order

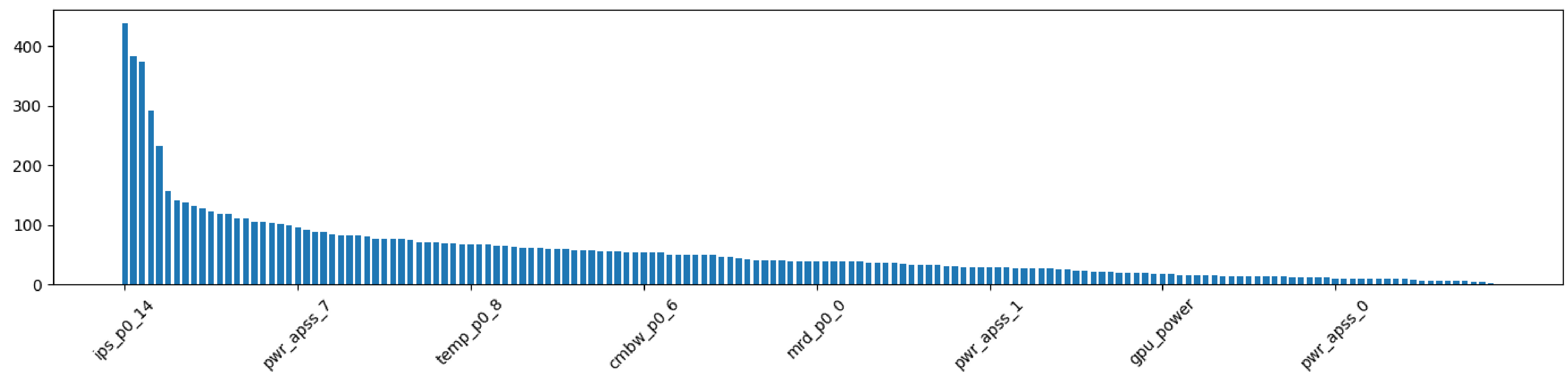
```
In [69]: last_mode_2 = hpcs.index[hpcs['anomaly']==2][-1]
         se.iloc[last_mode_2].sort_values(ascending=False)[:8]

Out[69]: ips_p0_14    1082.955690
         ips_p0_12     923.743869
         ips_p0_10     914.805579
         ips_p0_11     709.650840
         ips_p0_8      565.250761
         ips_p0_9      405.972020
         ips_p0_13     267.835655
         pwr_p0_2      249.472900
         Name: 6666, dtype: float64
```

- Again, they are performance related

Multiple Signal Analysis

Here are the average errors for mode 1 anomalies

```
In [72]: mode_1 = hpcs.index[hpcs['anomaly']==1]
         tmp =  se.iloc[mode_1].mean().sort_values(ascending=False)
         util.plot_bars(tmp, tick_gap=20, figsize=figsize)
```

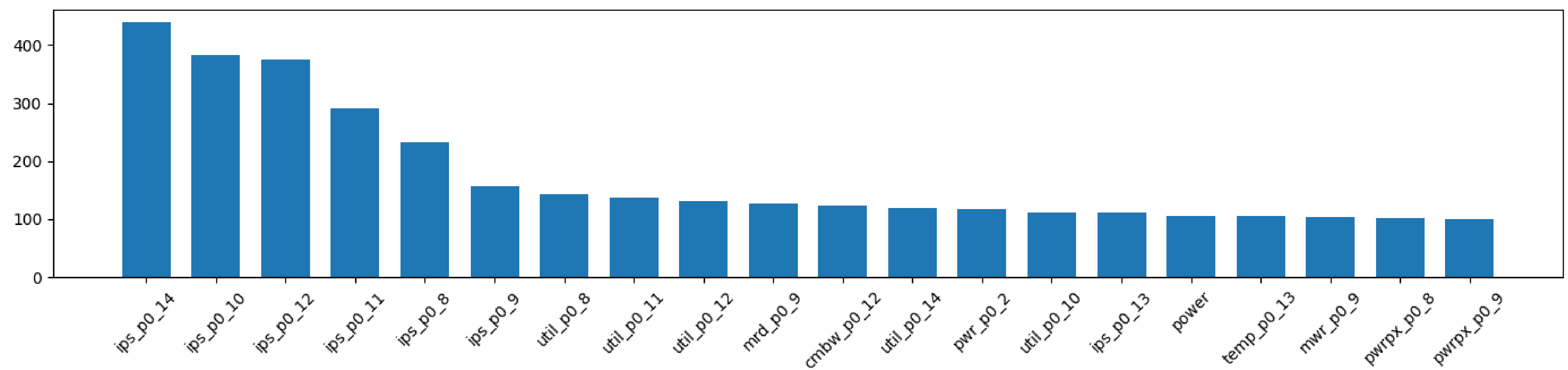


- Errors are concentrated on a small number of features

Multiple Signal Analysis

These are the 20 largest average errors for mode 1 anomalies

In [74]:
```
mode_1 = hpcs.index[hpcs['anomaly']==1]
tmp =  se.iloc[mode_1].mean().sort_values(ascending=False)
util.plot_bars(tmp.iloc[:20], figsize=figsize)
```

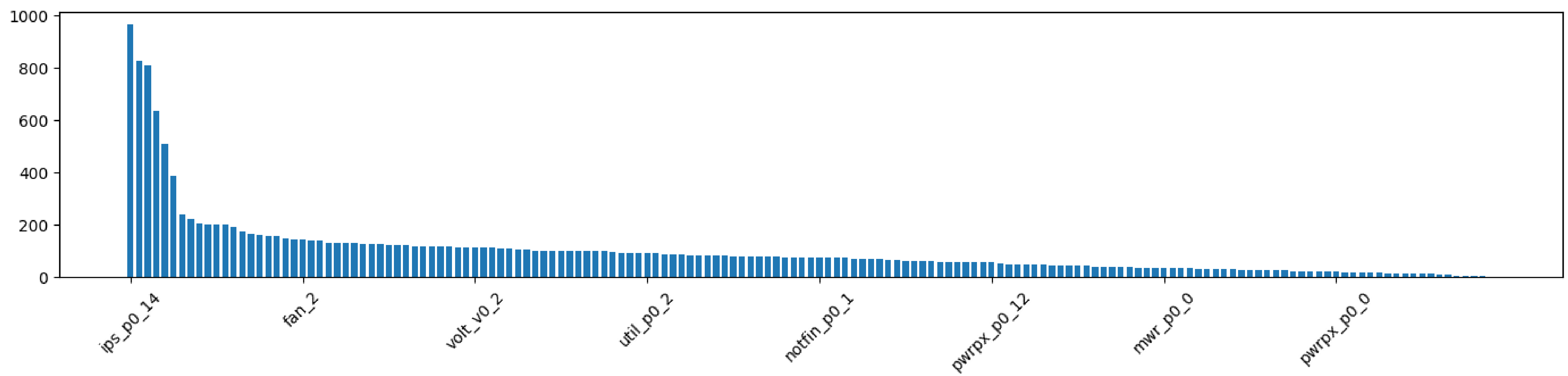


- The largest errors are on "ips", then on "util" (utilization)

Multiple Signal Analysis

Let's repeat the analysis for mode 2. Here are the average errors

```
In [75]: mode_2 = hpcs.index[hpcs['anomaly']==2]
         tmp =  se.iloc[mode_2].mean().sort_values(ascending=False)
         util.plot_bars(tmp, tick_gap=20, figsize=figsize)
```

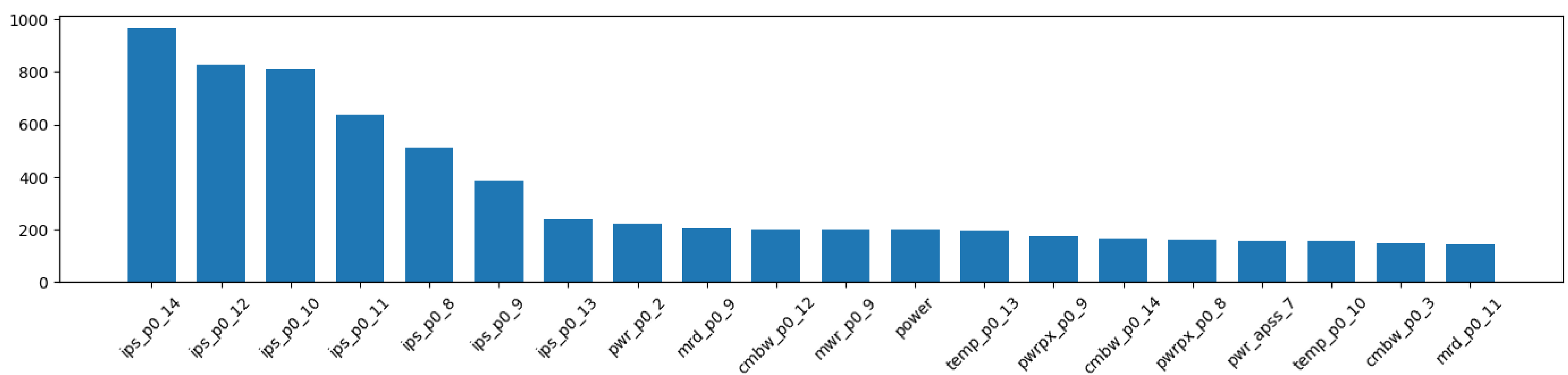


- The situation is similar to mode 1

Multiple Signal Analysis

The 20 largest average errors for mode 2

In [76]:
```
mode_2 = hpcs.index[hpcs['anomaly']==2]
tmp =  se.iloc[mode_2].mean().sort_values(ascending=False)
util.plot_bars(tmp.iloc[:20], figsize=figsize)
```



- The largest errors are on "ips", then on power signals

Considerations

Autoenders can be used for anomaly detection

- The provide the usual benefits of Neural Networks
  - E.g. scalability, limited overfitting, limited need for preprocessing
- They tend to be more reliable than autoregressors
- They provide more fine grained information than density estimation
- ...And you can make them deep!

Analyzing individual efforts provides clues about the anomalies

- In this case, we manage to focus on 10-20 features, rather than 160!

Density estimation is (usually) a bit better at pure anomaly detection

- ...But there is no reason not to use both approaches!
- E.g. density estimation for detection, autoencoders for the analysis