In [1]:
```
# ============================================================
# Notebook setup: run this before everything
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(15, 4.5)

from sklearn.model_selection import GridSearchCV
from util import util
import numpy as np
from matplotlib import pyplot as plt
import pandas as pd
import os

# Load data
data_file = os.path.join('..', 'data', 'hpc.csv')
hpc = pd.read_csv(data_file, parse_dates=['timestamp'])

# Identify input columns
inputs = hpc.columns[1:-1]
ninputs = len(inputs)
```

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 a tensor x and the output *should be similar* to the same tensor x

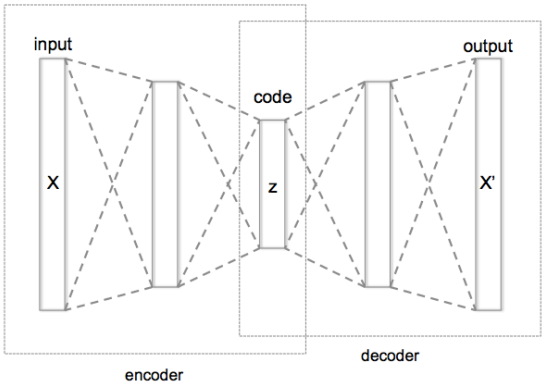


Figure from Wikipedia

Autoencoders

Autoencoders can be broken down in two halves

- An encoder, i.e. $e(x, \theta_e)$, mapping x into a vector of *latent variables* z
- A decoder, i.e. $d(z, \theta_d)$, mapping z into reconstructed input tensor

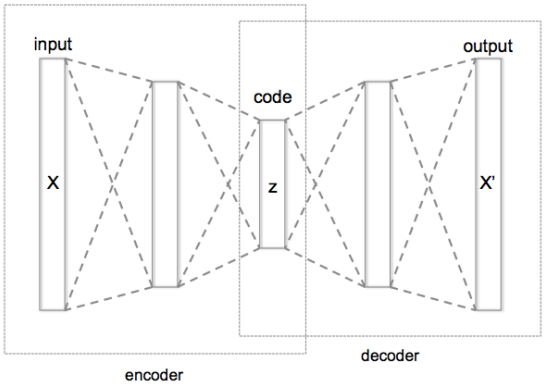


Figure from Wikipedia

Training an Autoencoder

Autoencoders are typically trained for minimum MSE:

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

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

A nice tutorial about autoencoders can be found on the Keras blog

There is a risk that an autoencoder learns a trivial transformation ($x' = x$)

This is obviously undesired, and it can be avoided by:

- Choosing a small-dimensional latent space (*compressing* autoencoder)
- By encouraging sparse encodings with an L1 regularizer (*sparse* autoencoder)

Autoencoders for Anomaly Detection

Autoencoders can be used for anomaly detection

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

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

This approach has some PROs and CONs compared to KDE

- The *size of a Neural Network* does not depend on the size of the training set
- Neural Networks have good *support for high dimensional data*

- ...Plus *limited overfitting* and *fast prediction/detection time*
- However, input reconstruction can be *harder than density estimation*

Let's prepare the data to test the approach

Shall we standardize/normalize the data? And why?

NNs and Standardization

Normalization is important for NNs, due to the use of *gradient descent*

The performance of SGD depends a lot on its starting point

- DL libraries all come with robust weight initialization procedures
  - ...And robust default parameters for the gradient descent algorithms
- ...But those are designed for data that is:
  - Reasonably *close to zero*
  - Mostly *contained in a* $[-1, 1]^n$ *box*

You *can* use NNs with non standardize data

...But expect *far less reliable* results

- In addition, vector output should *always* be standardized/normalized
- We'll see why in a short while

Data Preparation

We'll prepare our data as we did for KDE

First we apply a standardization step:

In [2]:
```
tr_end, val_end = 3000, 4500
hpcs = hpc.copy()
tmp = hpcs.iloc[:tr_end]
hpcs[inputs] = (hpcs[inputs] - tmp[inputs].mean()) / tmp[inputs].std()
```

The we separate a training, validation, and test set

In [3]:
```
trdata = hpcs.iloc[:tr_end]
valdata = hpcs.iloc[tr_end:val_end]
tsdata = hpcs.iloc[val_end:]
```

Building an Autoencoder

The we can build an autoencoder (we'll use tensorflow 2.0 and keras)

First, we build the model using (e.g.) the functional API

In [4]:
```
import keras
from keras import layers, callbacks

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)
```

- `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 can prepare our model for training

In keras terms, we *compile* it

In [5]:
```
ae.compile(optimizer='Adam', loss='mse')
```

- We are using the `Adam` optimizer (a variant of Stochastic Gradient Descent)

Then we can start training:

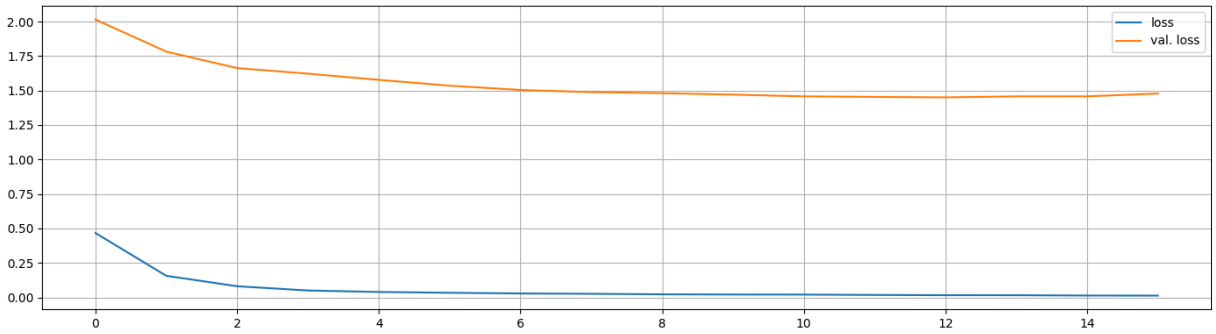
In [6]:
```
cb = [callbacks.EarlyStopping(patience=3, restore_best_weights=True)]
history = ae.fit(trdata[inputs], trdata[inputs], validation_split=0.1,
                 callbacks=cb, batch_size=32, epochs=30, verbose=0)
```

- 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 [7]:
```
util.plot_training_history(history, figsize=figsize)
```



Autoencoders in Keras

Finally, we can obtain the predictions

In [8]:
```
preds = pd.DataFrame(index=hpcs.index, columns=inputs, data=ae.predict(hpcs[
preds.head()
```

Out[8]:

	ambient_temp	cmbw_p0_0	cmbw_p0_1	cmbw_p0_10	cmbw_p0_11	cmbw_p0_12
0	0.241862	-0.570220	0.847816	1.652688	1.837251	2.104128
1	-0.820812	-0.729523	-0.156566	2.290839	2.074515	2.243163
2	-0.964374	-0.903323	-0.119433	2.409608	2.406907	2.284556
3	-0.915004	-0.859950	-0.642845	2.401014	2.278951	2.273461
4	-1.003353	-0.851472	-0.484362	2.302497	2.254762	2.266041

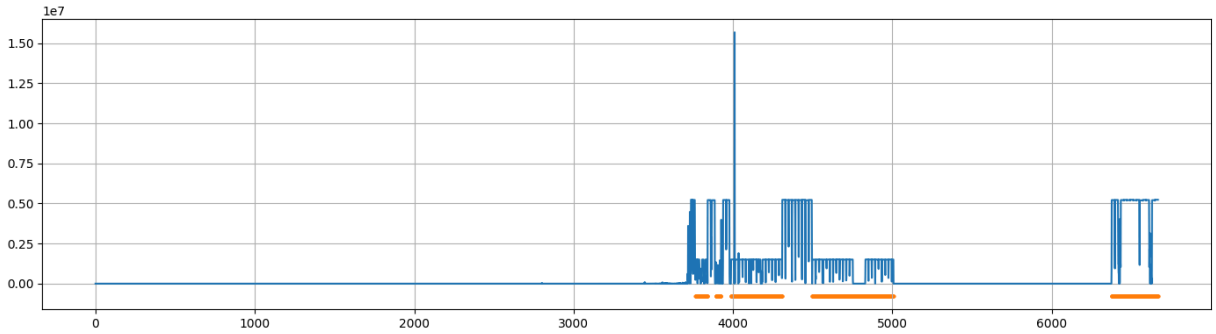
5 rows × 159 columns

- These are the reconstructed values for all the input features

Alarm Signal

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

In [9]:
```
labels = pd.Series(index=hpcs.index, data=(hpcs['anomaly'] != 0), dtype=int)
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)
```



> **This is very similar to the KDE and GMM signal: why?**

Semantic of Neural Regressors

Let's try to understand what we have just done

When we train an autoencoder (renamed here as h), we solve:

$$\arg\min_{\theta} \|h(x,\theta) - x\|_2^2$$

By expanding the L2 norm, we get:

$$\arg\min_{\theta} \sum_{i=1}^{m}\sum_{j=1}^{n} \left(h_j(x_i,\theta) - x_{i,j}\right)^2$$

By introducing a $\log$ and $\exp$ transformation we obtain:

$$\arg\min_{\theta} \log\exp\left(\sum_{i=1}^{m}\sum_{j=1}^{n} \left(h_j(x_i,\theta) - x_{i,j}\right)^2\right)$$

Semantic of Neural Regressors

Then, from the last step:

$$\arg\min_{\theta} \log\exp\left(\sum_{i=1}^{m}\sum_{j=1}^{n} \left(h_j(x_i,\theta) - x_{i,j}\right)^2\right)$$

We rewriting the outer sum using properties of exponentials:

$$\arg\min_{\theta} \log\prod_{i=1}^{m}\exp\left(\sum_{j=1}^{n} \left(h_j(x_i,\theta) - x_{i,j}\right)^2\right)$$

Then we rewrite the inner sum in matrix form:

$$\arg\min_{\theta} \log \prod_{i=1}^{m} \exp\left(\left(h(x_i, \theta) - x_{i,j}\right)^T I \left(h(x_i, \theta) - x_{i,j}\right) \right)$$

Semantic of Neural Regressors

Starting from the last step:

$$\arg\min_{\theta} \log \prod_{i=1}^{m} \exp\left(\left(h(x_i, \theta) - x_{i,j}\right)^T I \left(h(x_i, \theta) - x_{i,j}\right) \right)$$

We make a few adjustment that do not change the optimal solution:

- We negate the argument of $\exp$ and swap the $\arg\min$ for a $\arg\max$
- We multiply exponent by $1/2\sigma$ (for some constant σ)
- We multiply the exponential by $1/\sqrt{2\pi}\sigma$

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

Semantic of Neural Regressors

Let's look at our last formulation:

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

The term inside the product is the PDF of a multivariate normal distribution

$$\arg\max_{\theta} \log \prod_{i=1}^{m} f\left(x_i, h(x_i), \sigma I\right)$$

- In particular a distribution *centered on* $h(x_i)$
- ...With *independent Normal components*
- ...All having *uniform variance*

Semantic of Neural Regressors

Let's discuss some implications

When we use a MSE loss, we are *training for maximum likelihood*

- ...Just like density estimators!
- This is actually true for *many* ML approaches

The *output* of a (MSE trained) regressor has a *probabilistic interpretation*

- Specifically, the output is the *mean of a conditional distribution*
- The distribution represents the *variability of the target*
- ...Once the effect of the input is taken into account
- Another way to think of it: *noise* around the prediction

Semantic of Neural Regressors

Let's discuss some implications

We are implicitly assuming that the *noise is normally distributed*

- This true in many cases, but not always
- E.g., sometimes large values are under-represented
- ....Leading to log-normal distributions
- In this cases, applying a log transformation to the output can be very effective

We are also assuming that the all output components *have the same variance*

- This is another (very) good reason to standardize the output

Semantic of Neural Regressors

Let's discuss some implications

We are also assuming that the *noise on all output components is independent*

- This might be true even if the output components themselves are correlated
- ...But still it is not true in all cases

All these implicit assumption can make the problem *harder*

- This is why error reconstruction can be harder than density estimation

Finally, our *alarm signal* can be interpreted as a *density*:

- To see why, just apply the transformation to $\|x - d(e(x, \theta_e), \theta_d)\|_2^2$
- This fact explains why the signal is similar to the KDE one

Threshold Optimization

The threshold can be optimized as usual

In [10]:
```
c_alarm, c_missed, tolerance = 1, 5, 12
cmodel =  util.HPCMetrics(c_alarm, c_missed, tolerance)
th_range = np.linspace(1e4, 2e5, 200)

th_ae, val_cost_ae = util.opt_threshold(signal_ae[tr_end:val_end], hpcs['anc
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_
print(f'Cost on the test set: {ts_cost_ae}')
```

```
Best threshold: 124572.864
Cost on the training set: 0
Cost on the validation set: 263
Cost on the test set: 265
```

- The performance is similar to KDE (not surprisingly)

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

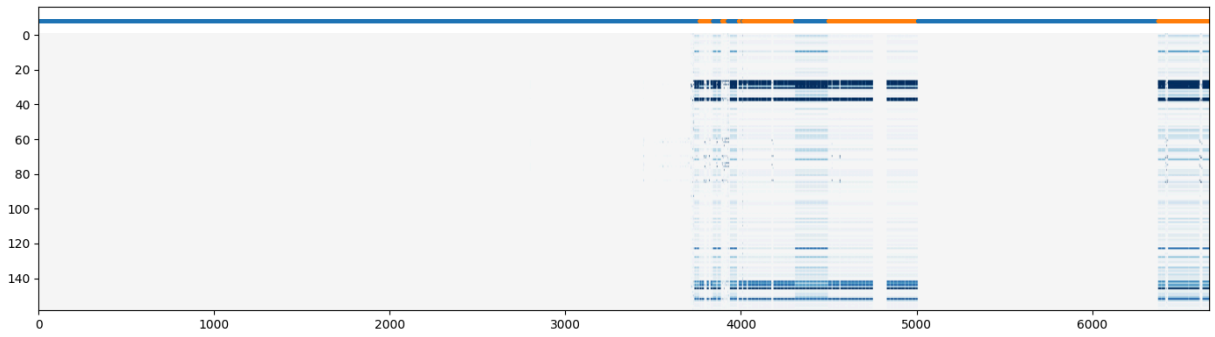
In [11]:
```
se = np.square(preds - hpcs[inputs])
signals_ae = pd.DataFrame(index=hpcs.index, columns=inputs, data=se)
util.plot_dataframe(signals_ae, labels, vmin=-5e4, vmax=5e4, figsize=figsize
```

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*

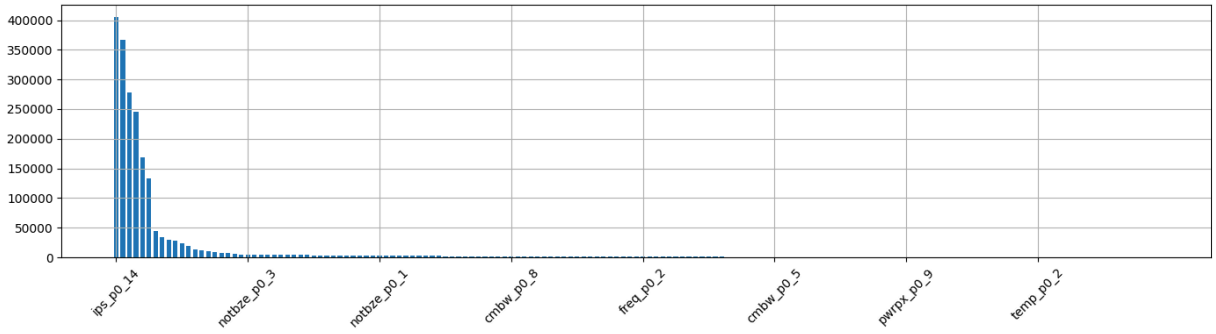
In [12]:
```
se = np.square(preds - hpcs[inputs])
signals_ae = pd.DataFrame(index=hpcs.index, columns=inputs, data=se)
util.plot_dataframe(signals_ae, labels, vmin=-5e4, vmax=5e4, figsize=figsize
```



Multiple Signal Analysis

Here are the *average errors* for all anomalies (sorted by decreasing value)

In [13]:
```
mode_1 = hpcs.index[hpcs['anomaly'] != 0]
tmp =  se.iloc[mode_1].mean().sort_values(ascending=False)
util.plot_bars(tmp, tick_gap=20, figsize=figsize)
```

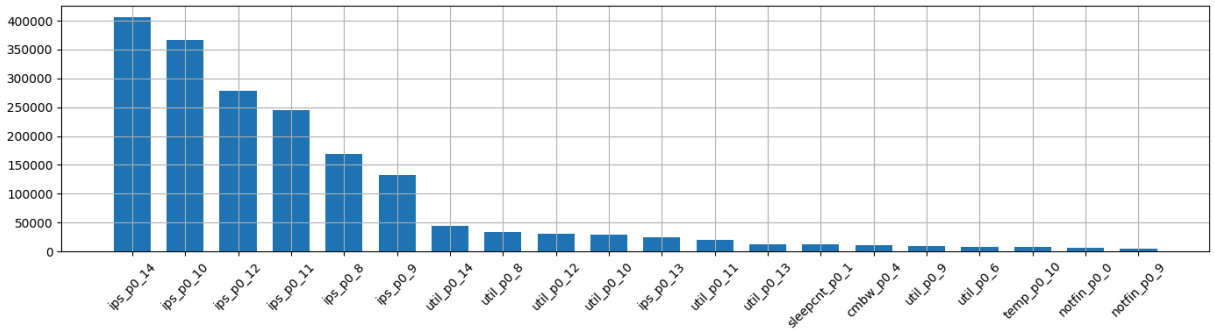


- Errors are concentrated on 10-20 features

Multiple Signal Analysis

These are the 20 *largest* average errors for all anomalies

In [14]:
```
mode_1 = hpcs.index[hpcs['anomaly'] != 0]
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)
- This kind of information can be *very valuable* for a domain expert!