Baseline Approach

Train/Test Split

We'll try to detect the component state by learning an autoencoder

- We'll train a model on the earlier data
- ...And then use the reconstruction error as a proxy for component wear

We start as usual by splitting the training and test set

In [3]:
```
tr_sep = int(0.5 * len(data_b))
data_b_tr = data_b.iloc[:tr_sep]
data_b_ts = data_b.iloc[tr_sep:]
```

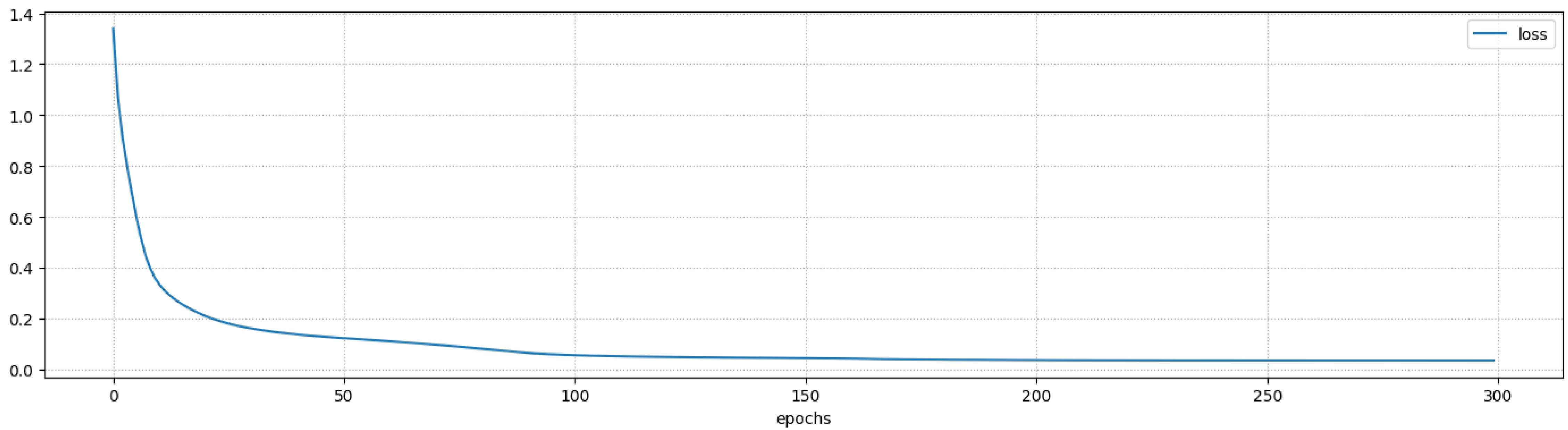
...And then by standardizing our data

In [4]:
```
scaler = StandardScaler()
data_b_s_tr = scaler.fit_transform(data_b_tr)
data_b_s_ts = scaler.transform(data_b_ts)
data_b_s = pd.DataFrame(columns=data_b.columns, data=np.vstack([data_b_s_tr, data_b_s_ts]))
```

Training and Autoencoder

Now we can build and train the autoencoder

In [13]:
```
nn = util.build_nn_model(input_shape=len(data_b.columns), output_shape=len(data_b.columns),
                         hidden=[len(data_b.columns)//2])
history = util.train_nn_model(nn, data_b_s_tr, data_b_s_tr, loss='mse', validation_split=0.0,
                              batch_size=32, epochs=300)
util.plot_training_history(history, figsize=figsize)
```



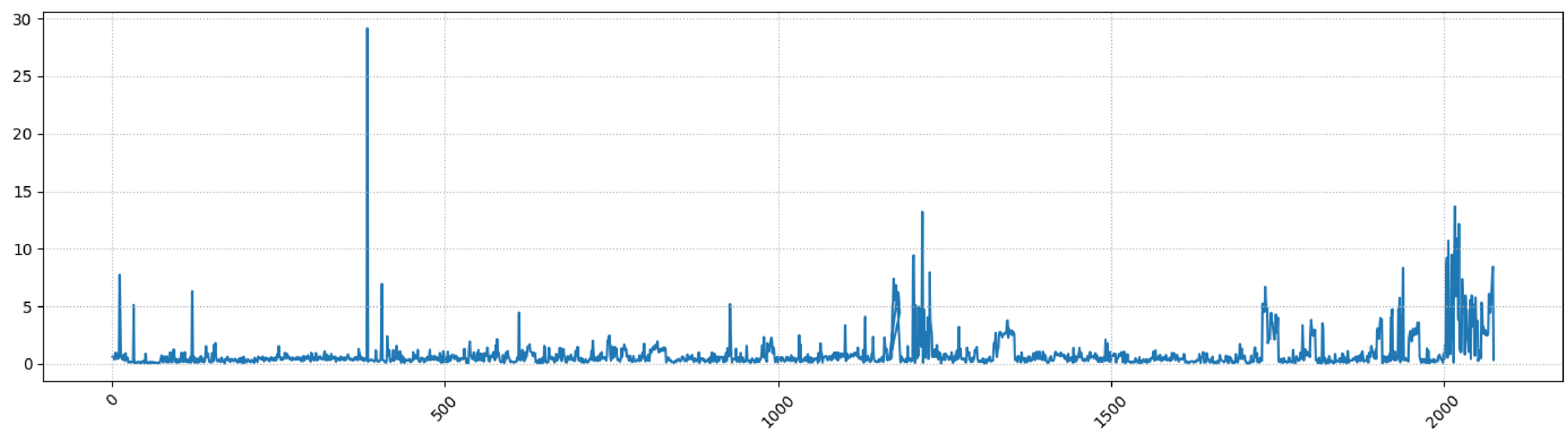

```
Final loss: 0.0346 (training)
```

- We need many epochs to compensate for the small number of samples

Evaluation

Let's check the reconstruction error

```
In [14]: pred = nn.predict(data_b_s, verbose=0)
         se = (data_b_s - pred)**2
         sse = pd.Series(index=data_b.index, data=np.sum(se, axis=1))
         util.plot_series(sse, figsize=figsize)
```

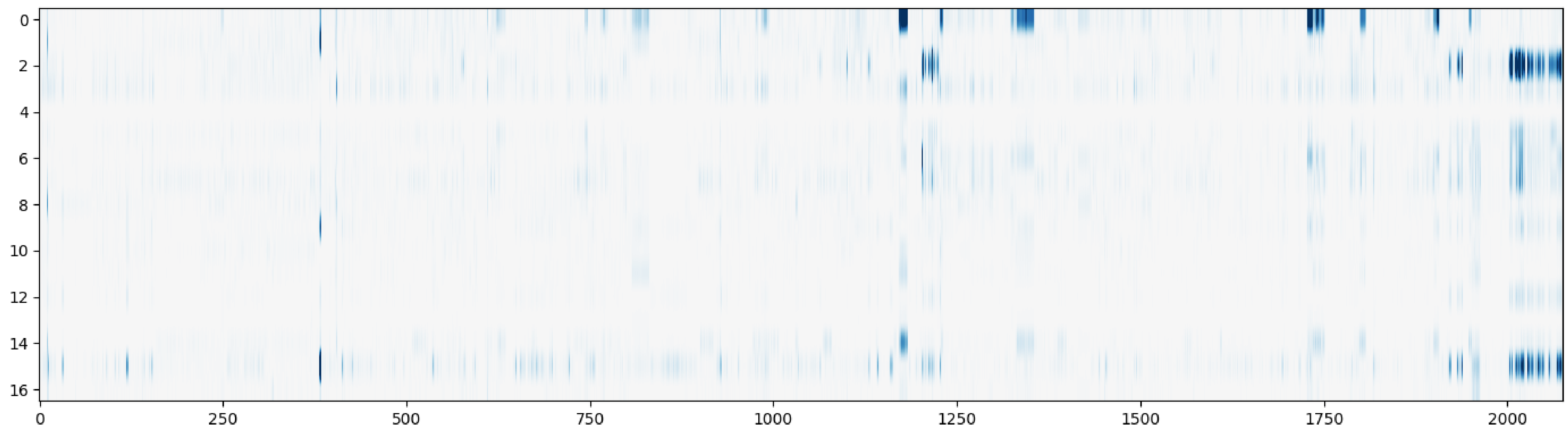


- Since we have a single run, we will limit ourselves to a visual inspection
- ...And the signal does not look very clear

Evaluation

We can gain more information by checking the individual errors

In [15]:
```
util.plot_dataframe(se, figsize=figsize)
```



- Reconstruction errors are large for different features over time

Do you think we can improve these results? How?

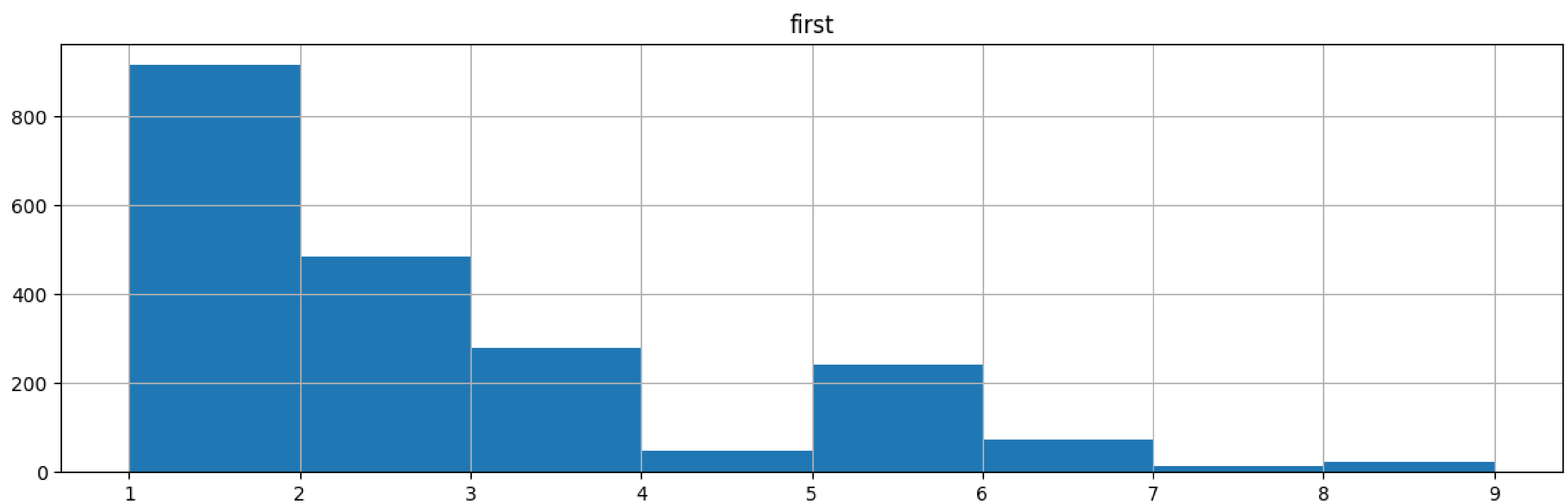
Altering the Training Distribution

Distribution Discrepancy

A major problem is related to the distribution balance

The modes of operation are not used equally often

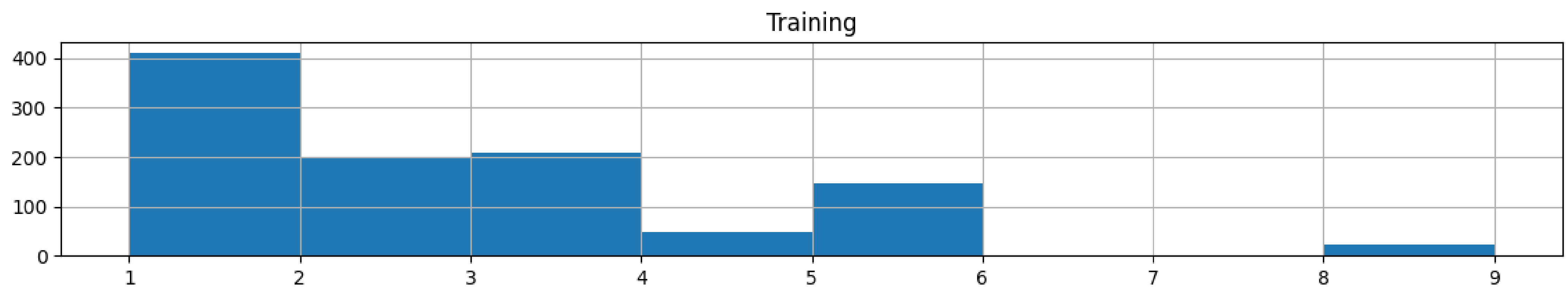
In [16]:
```
data_b['mode'].hist(figsize=figsize, bins=np.arange(1, 10));
```

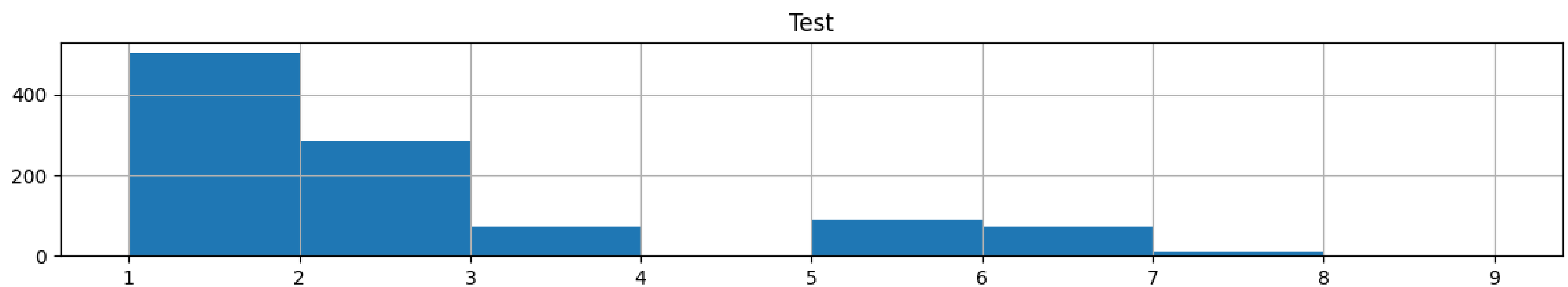


Distribution Discrepancy

In fact, there is a difference between the training and test distribution

In [17]:
```
data_b_tr['mode'].hist(figsize=(figsize[0], figsize[1]/2), bins=np.arange(1, 10)); plt.title('Tr
data_b_ts['mode'].hist(figsize=(figsize[0], figsize[1]/2), bins=np.arange(1, 10)); plt.title('Te
```





Maximum Likelihood

This matters because we are training for maximum likelihood

...Ideally we would like to solve:

$$\mathop{\mathrm{argmax}}_{\theta} \mathbb{E}_{\hat{x},\hat{y}\sim P}\left[\prod_{i=1}^{m} f_\theta(\hat{y}_i \mid \hat{x}_i)\right]$$

- P represents the real (joint) distribution
- $f_\theta(\cdot \mid \cdot)$ is our model, with parameter vector θ
- I.e. an estimator for a conditional distribution
- We distinguish $\hat{x}$ (input) and $\hat{y}$ (output) to cover generic supervised learning
- ...Even if for an autoencoder they are the same

...And Empirical Risk

...But in practive we don't have access to the full distribution

So we use Monte-Carlo approximation:

$$\operatorname*{argmax}_{\theta} \prod_{i=1}^{m} f_\theta(\hat{y}_i \mid \hat{x}_i)$$

- Typically, we consider a single sample $\hat{x}, \hat{y}$ (i.e. the training set)
- The resulting objective (i.e. the big product) is sometimes called empirical risk

This the usual training approach with most ML models, and it mostly works

Problems arise when our sample is biased. E.g. because:

- We can collect data only under certain circumstances
- The dataset is the result of a selection process
- ...Or perhaps due to pure sampling noise

Handling Sampling Noise

So, let's recap

- Our problem is that the training sample is biased
- ...So that it is not representative of the true distribution

How can we deal with this problem?

Handling Sampling Noise

So, let's recap

- Our problem is that the training sample is biased
- ...So that it is not representative of the true distribution

How can we deal with this problem?

- A possible solution would be to alter the training distribution
- ...So that it matches more closely the test distribution

...And this is actually something we can do!

- E.g. we can use data augmentation
- ...Or we can use sample weights

Handling Sampling Noise with Sample Weights

Let our training set consist of $\{(\hat{x}_1, \hat{y}_1), (\hat{x}_2, \hat{y}_2)\}$

The corresponding optimization problem would be:

$$\operatorname*{argmax}_{\theta} f_\theta(\hat{y}_1 \mid \hat{x}_1) f_\theta(\hat{y}_2 \mid \hat{x}_2)$$

Let's pretend that sample #2 occurs twice; that would lead to:

$$\operatorname*{argmax}_{\theta} f_\theta(\hat{y}_1 \mid \hat{x}_1) f_\theta(\hat{y}_2 \mid \hat{x}_2)^2$$

In general, multiplicities show up as exponents in the training objective

$$\operatorname*{argmax}_{\theta} \prod_{i=1}^{m} f_\theta(\hat{y}_i \mid \hat{x}_i)^{n_i}$$

Handling Sampling Noise with Sample Weights

We can use this insight to simulate a different distribution

- In particular, assuming that $\tilde{p}_i$ is the true probability of sample i
- ...And that $\hat{p}_i$ is its probability in the training set

...Then we can simulate a training distribution closer to the true one by solving:

$$\operatorname*{argmax}_\theta \prod_{i=1}^m f_\theta(\hat{y}_i \mid \hat{x}_i)^{\tilde{p}_i/\hat{p}_i}$$

Switching to log scale (and minimization), we end up with sample weights

$$\operatorname*{argmin}_\theta - \sum_{i=1}^m \frac{\tilde{p}_i}{\hat{p}_i} \log f_\theta(\hat{y}_i \mid \hat{x}_i)$$

- We are still limited to examples in the training set, but this is a big improvement

Handling Sampling Noise with Sample Weights

The tricky part is making a good assumption about $\tilde{p}$

- A common one is just neutralizing sampling bias
- In practice, we assume $\tilde{p}_i = 1, \forall i = 1..m$
- ...And we compute $\hat{p}_i$ based on the training data

This is called inverse probability weighting

For example, if we are afraid some classes are under-represented

- ...Then we make $\hat{p}_i =$ the frequency of the class for example i
- ...Which is of course the typical "class rebalancing trick"

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But this is a general rule and we can do much more!

Handling Sampling Noise with Sample Weights

First, we are not limited to classes

- If we are afraid some operating modes are under-represented
- ...Then we make $\hat{p}_i =$ the frequency of the mode for example i

Second, we can exploit information about the test distribution

- If we can make reasonable assumptions about our $\tilde{p}_i$
- ...Then we know how to update the weights to take that into account

Third, we can deal with selection bias

- E.g. consider the problem of estimating success rates for organ transplants
- Subject in the training set will obviously not be chosen at random
- If we can estimate their selection probabilities $\hat{p}_i$ (e.g. via another classifier)
- ...Then we can mitigate the bias effect using sample weights

Handling Sampling Noise with Sample Weights

Fourth: we can handle bias over continuous attributes (e.g. income)

- Then we can compute $\hat{p}_i$ using (e.g.) a density estimator
- ...Or any other model capably of producing a probability as output

Just beware of overly large/small densities

...Since they will break havoc in numerical optimization algorithms

- Patch 1: apply (lower/upper) clipping to densities
- Patch 2: normalize densities over the training set (make them sum up to 1)

This means we can cancel (sampling) bias based on any kind of attribute

Handling Sampling Noise with Sample Weights

There's a final notable case in case our loss is the MSE

In this case we have proved the training problem is equivalent to:

$$\operatorname{argmin}_\theta - \sum_{i=1}^m \log k \exp\left(-\frac{1}{2}(\hat{y}_i - h_\theta(\hat{x}_i))^2\right)$$

- We have simply replaced the generic PDF with a Normal one
- We have $k = 1/\sqrt{2\pi}$ to simplify the notation

Let's now introduce sample weights, in the form as $1/\hat{\sigma}_i^2$

By doing so we get:

$$\operatorname{argmin}_\theta - \sum_{i=1}^m \frac{1}{\hat{\sigma}_i^2} \log k \exp\left(-\frac{1}{2}(\hat{y}_i - h_\theta(\hat{x}_i))^2\right)$$

Handling Sampling Noise with Sample Weights

Which can be rewritten as:

$$\operatorname*{argmin}_{\theta} - \sum_{i=1}^{m} \log k \exp\left(-\frac{1}{2}\left(\frac{\hat{y}_i - h_\theta(\hat{x}_i}{\hat{\sigma}_i^2}\right)^2\right)$$

- This means that sample weights with an MSE loss
- ...Can be interpreted as inverse sample variances

Handling Sampling Noise with Sample Weights

Which can be rewritten as:

$$\operatorname*{argmin}_{\theta} - \sum_{i=1}^{m} \log k \exp\left(-\frac{1}{2} \left(\frac{\hat{y}_i - h_\theta(\hat{x}_i}{\hat{\sigma}_i^2} \right)^2 \right)$$

- This means that sample weights with an MSE loss
- ...Can be interpreted as inverse sample variances

This gives us a way to account for measurement errors

- If we know that there is a measurment error with stdev $\hat{\sigma}_i$ on example i
- ...We can account for that by using $1/\hat{\sigma}_i^2$ as a weight

The result is analogous to using a separate variance model

Canceling Sampling Bias in Our Problem

Let's apply the approach to our skinwrapper example

- In our case, we observed there is a bias linked to operating modes
- We do not know the "true" distribution
- ...But is reasonable to try and be fair w.r.t. any operating mode

So we can open for the inverse probability weighting approach

First, we compute the inverse mode frequencies:

In [18]:
```
vcounts = data_b_tr['mode', 'first'].value_counts()
mode_weight = vcounts.sum() / vcounts
```

Then we compute the weight for each example:

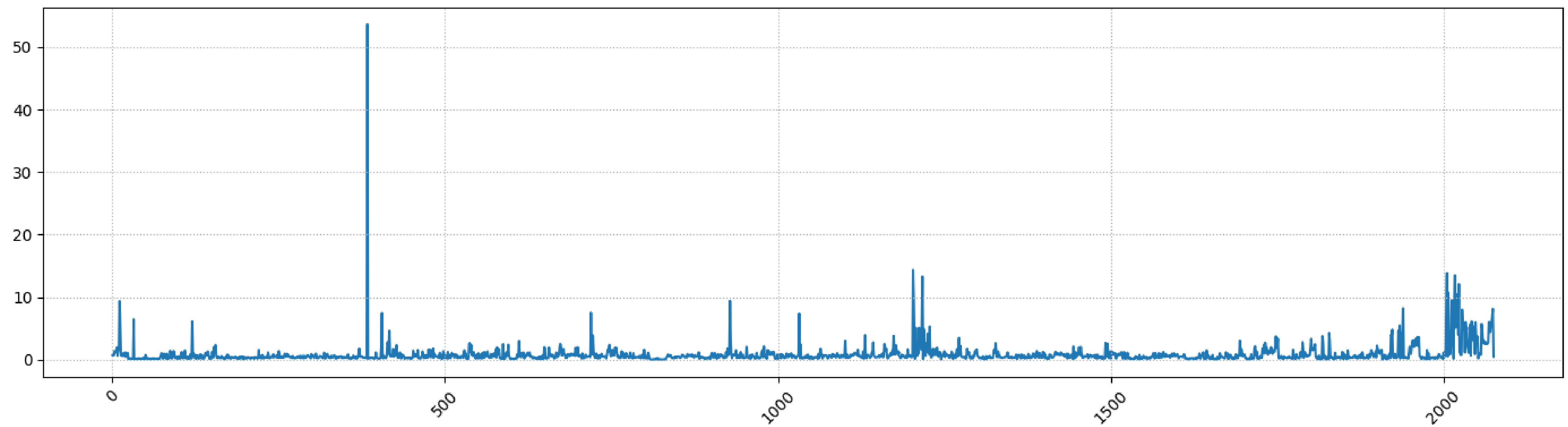
In [19]:
```
sample_weight = mode_weight[data_b_tr['mode', 'first']]
```

Training with Sample Weights

Evaluation

Let's check the new reconstruction error

```
In [21]: pred2 = nn2.predict(data_b_s, verbose=0)
         se2 = (data_b_s - pred2)**2
         sse2 = pd.Series(index=data_b.index, data=np.sum(se2, axis=1))
         util.plot_series(sse2, figsize=figsize)
```

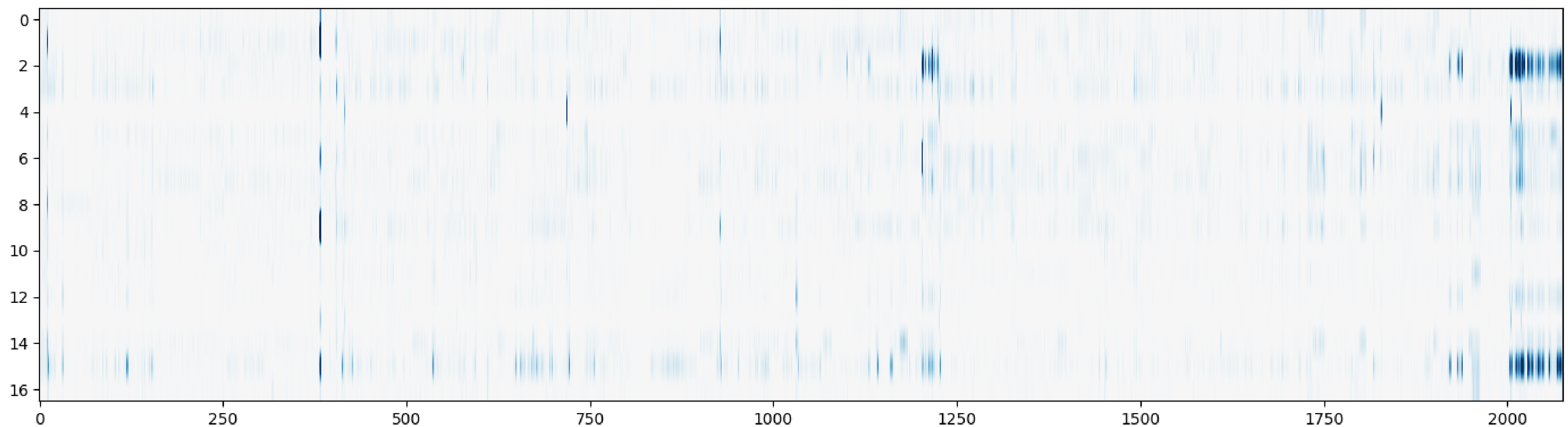


An intermediate peak has disappeared

Evaluation

...And the individual error components are very different

In [22]:
```
util.plot_dataframe(se2, figsize=figsize)
```



Now there is a much clearer plateau close to the end of the run