In [1]:
```python
# ============================================================
# Notebook setup
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(14, 4)

from util import util
import os
import pandas as pd
import numpy as np
from sklearn.preprocessing import StandardScaler
import warnings
warnings.simplefilter("ignore")
from matplotlib import pyplot as plt

# Specify datafile
data_file = os.path.join('..', 'data', 'vegashrinker.csv')
# Read data
data = pd.read_csv(data_file)
# Define the input feature
feat_in_r = data.columns[[0, 6, 7, 9, 11, 12, 13]]
# Apply binning
aggmap = {a: ['mean', 'std', 'skew'] for a in feat_in_r}
aggmap['mode'] = 'first'
aggmap['pSpintor::VAX_speed'] = 'first'
binsize = 512 # 2 seconds of measurements
bins = []
for sname, sdata in data.groupby('segment'):
    sdata['bin'] = sdata.index // binsize # Build the bin numbers
    tmp = sdata.groupby('bin').agg(aggmap) # Apply the aggregation functions
    bins.append(tmp)
data_b = pd.concat(bins)
```

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

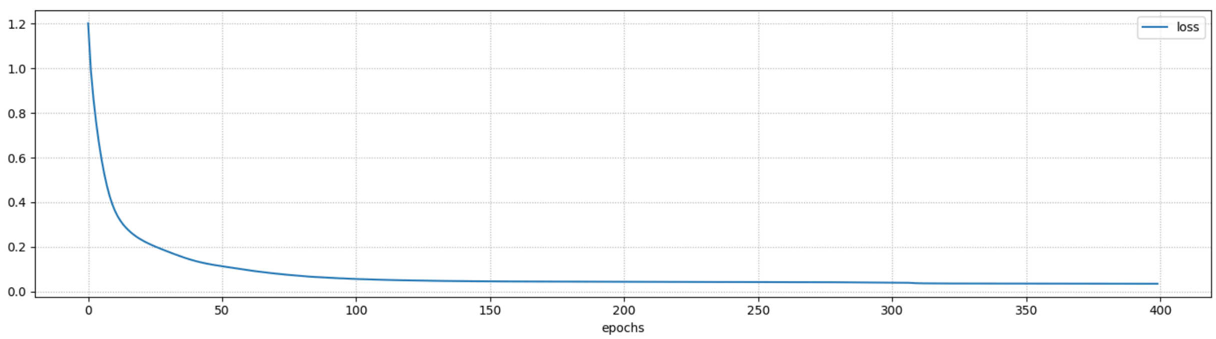
...And then by standardizing our data

```
In [3]: 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,
```

Training and Autoencoder

Now we can build and train the autoencoder

```
In [4]: nn = util.build_nn_model(input_shape=(len(data_b.columns),), output_shape=le
                                 hidden=[len(data_b.columns)//2])
history = util.train_nn_model(nn, data_b_s_tr, data_b_s_tr, loss='mse', vali
                                 batch_size=32, epochs=400)
util.plot_training_history(history, figsize=figsize)
```



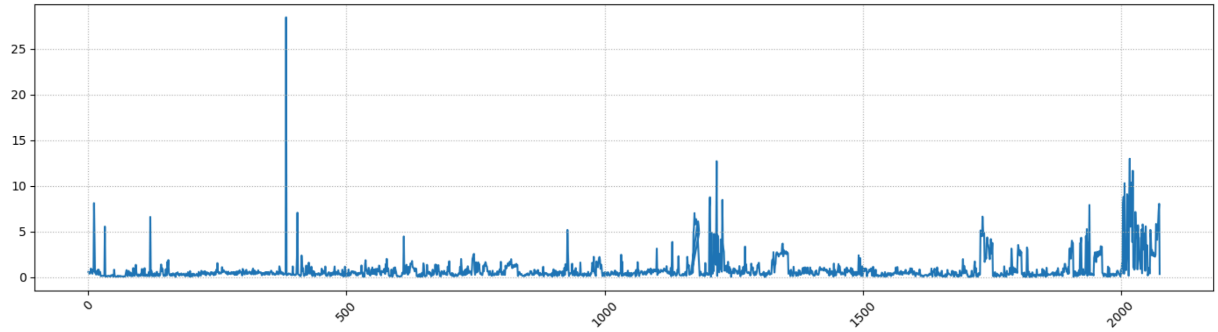

```
Final loss: 0.0346 (training)
```

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

Evaluation

Let's check the reconstruction error

```
In [5]: 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)
```

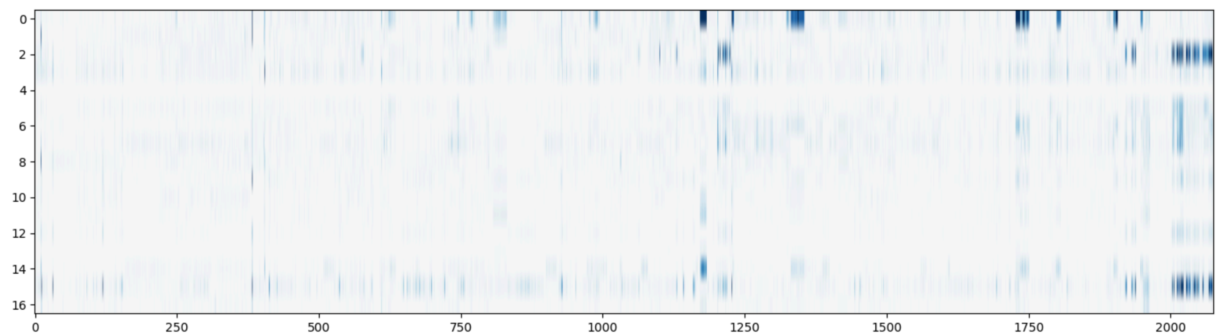


* Since we have a single run, we will limit ourselves to a visual inspection
* ...And the signal does not look very clear

Evaluation

We can gain more information by checking the individual errors

In [6]:
```
util.plot_dataframe(se, figsize=figsize)
```



* Reconstruction errors are large for different features over time

Do you think we can improve these results? How?

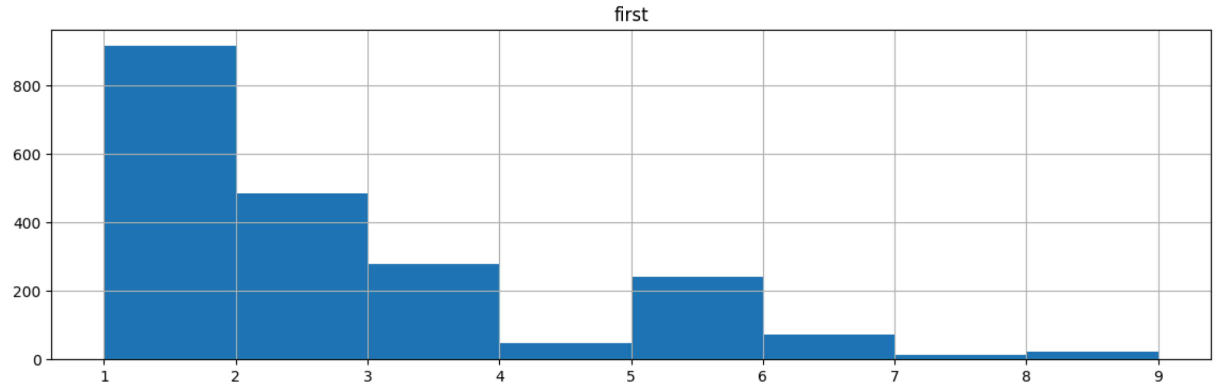
Altering the Training Distribution

Distribution Discrepancy

A major problem is related to the distribution balance

The modes of operation are *not used equally often*

In [7]:
```
data_b['mode'].hist(figsize=figsize, bins=np.arange(1, 10));
```

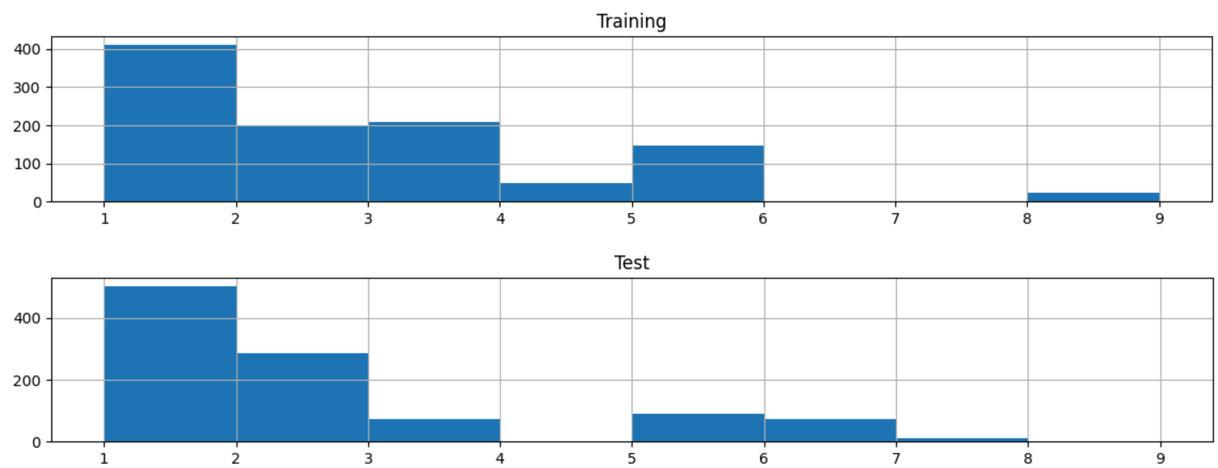


- Moreover, the mode of operation is a *controlled variable*
- ...Hence its distribution might change a lot based on the workload

Distribution Discrepancy

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

In [8]:
```
data_b_tr['mode'].hist(figsize=(figsize[0], figsize[1]/2), bins=np.arange(1,
data_b_ts['mode'].hist(figsize=(figsize[0], figsize[1]/2), bins=np.arange(1,
```



Maximum Likelihood

This matters because we are *training for maximum likelihood*

...Ideally we would like to solve:

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

- P represents the real (joint) distribution
- $f_\theta(\cdot \mid \cdot)$ is our estimated probability, with parameter vector θ
- I.e. an estimator for a conditional distribution

- We distinguish x (input) and y (output) to cover generic supervised learning
- ...Even if for an autoencoder they are the same

...And Empirical Risk

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

So usually we employ a Monte-Carlo approximation:

$$\operatorname*{argmax}_\theta \prod_{i=1}^m f_\theta(y_i \mid x_i)$$

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

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 issue 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 subsampling
- ...Or we can use *sample weights*

Virtual Alterations to the Training Distribution

Let our training set consist of $\{(x_1, y_1), (x_2, y_2)\}$

The corresponding optimization problem would be:

$$\underset{\theta}{\operatorname{argmax}}\, f_\theta(y_1 \mid x_1) f_\theta(y_2 \mid x_2)$$

If sample #2 occurred twice in the training data, we would have

$$\underset{\theta}{\operatorname{argmax}}\, f_\theta(y_1 \mid x_1) f_\theta(y_2 \mid x_2)^2$$

Normalizing over the number of samples does not change the minima:

$$\underset{\theta}{\operatorname{argmax}}\, f_\theta(y_1 \mid x_1)^{\frac{1}{3}} f_\theta(y_2 \mid x_2)^{\frac{2}{3}}$$

Virtual Alterations to the Training Distribution

Let's generalize these considerations:

A general training problem based on Empirical Risk Minimization is the form:

$$\underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} f_\theta(y_i \mid x_i)$$

We can virtually *alter the training distribution* via exponents:

$$\underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{m} f_\theta(y_i \mid x_i)^{w_i}$$

- We can do this to make the training distribution *more representative*
- E.g. when we expect a discrepancy between the training and test distribution

Virtual Distribution and Sample Weights

When we switch to log-likelihood minimization

...The exponents become *sample weights*

$$\underset{\theta}{\operatorname{argmin}} - \sum_{i=1}^{m} w_i \log f_\theta(y_i \mid x_i)$$

We can *always* view the weights as the ratio of two probabilities:

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

- p_i is the sampling bias that we want to *cancel*
- p_i^* is the distribution we wish to *emulate*

This approach is known as *importance sampling*

Canceling Sampling Bias in Our Problem

Let's apply the approach to our skinwrapper example

We know there's an *unwanted sampling bias* for some modes of operation

- Let $m(x_i)$ be the mode of operation for the i-th sample
- Then we can estimate p_i as a frequency of occurrence:

$$p_i = \frac{1}{n}|\{k : m(x_k) = m(x_i), k = 1..n\}|$$

We *don't want* out anomaly detector to be sensitive to the mode

- So we can assumption a uniform distribution for p_i^*:

$$p_i^* = \frac{1}{n}$$

Canceling Sampling Bias in Our Problem

By combining the two we get:

$$w_i = \frac{1}{|\{k : m(x_k) = m(x_i), k = 1..n\}|}$$

- I.e. the weight is just the inverse of the corresponding mode count

We can compute the weigths by first obtaining inverse counts for all modes

In [9]:
```
vcounts = data_b_tr['mode', 'first'].value_counts()
mode_weight = 1 / vcounts
```

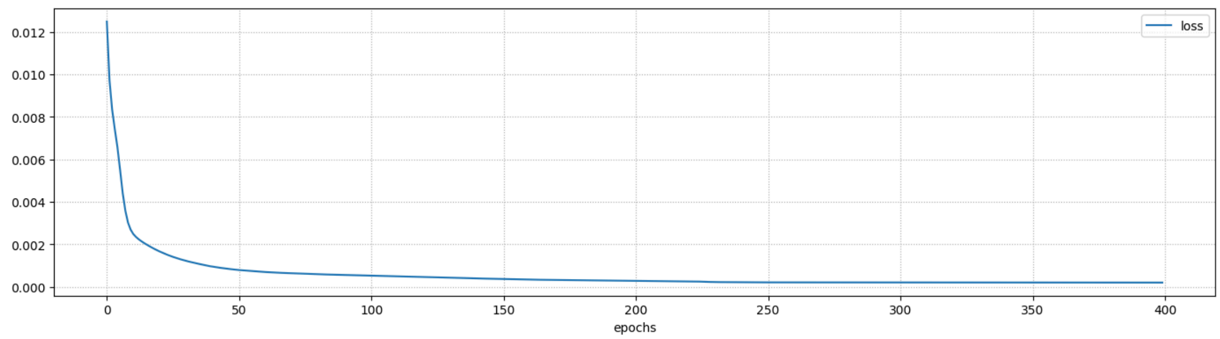
Then by associating the respective value to every sample:

In [10]:
```
sample_weight = mode_weight[data_b_tr['mode', 'first']]
```

Training with Sample Weights

Now we can pass training weights to the training algorithm

In [11]:
```
nn2 = util.build_nn_model(input_shape=(len(data_b.columns),), output_shape=l
history = util.train_nn_model(nn2, data_b_s_tr, data_b_s_tr, loss='mse', val
util.plot_training_history(history, figsize=figsize)
```

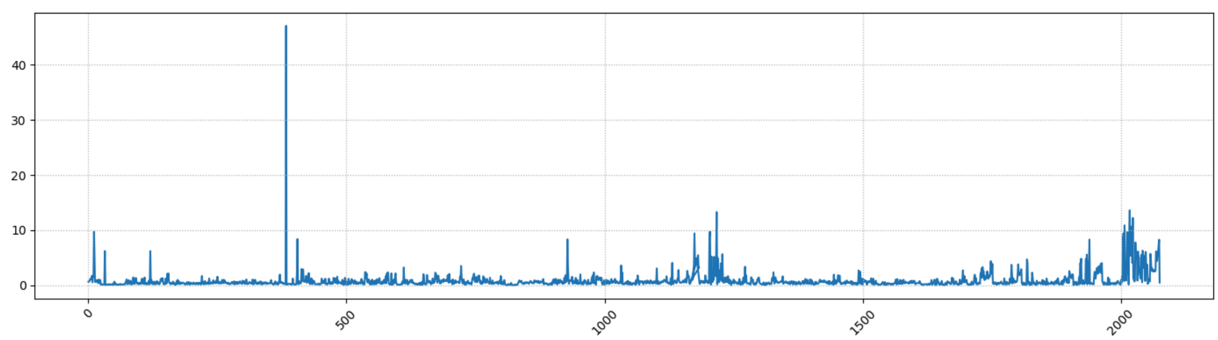



```
Final loss: 0.0002 (training)
```

Evaluation

Let's check the new reconstruction error

In [12]:
```
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)
```

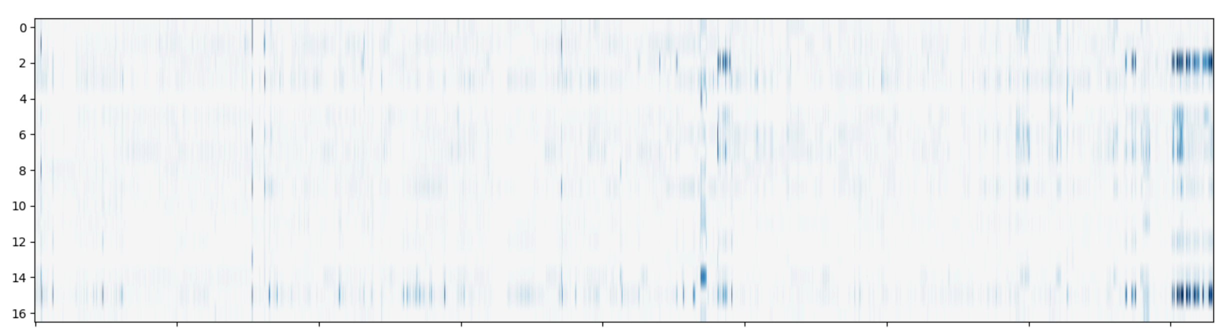


At a first glance, the change is not dramatic

Evaluation

...But the individual error components are very different

In [13]:
```
util.plot_dataframe(se2, figsize=figsize)
```



- Suspected anomalies in the middle sequence have almost disappeared

* ...And there is a much clearer plateau at the end of the signal

Applications of Importance Sampling

Despite its simplicity, importance sampling has many applications

Can you identify a few?

Class Rebalancing

The usual *class rebalancing trick* is a subcase of importance sampling

In this situation, we assume that some classes are over/under sampled

* Therefore, we estimate p_i using the class frequency
* We make a neutral (uniform) assumption on p_i^*
* ...And we define the sample weights for (x_i, y_i) as:

$$w_i = \frac{1}{n} \frac{n}{|\{k : y_k = y_i, k = 1..n\}|}$$

Watch out during evaluation!

* Evaluating via (e.g.) accuracy on the unmodified test set *might be a mistake*
* ...Since the weights alter the training distribution

Use a *cost model* instead, or just a confusion matrix

Removing Sampling Bias based on Continuous Attribute

The p_i and p_i^* values can be probability *densities*

...Meaning we can remove sampling bias over *continuous attributes*, e.g.:

* Continuous control variables (position, speed, etc.) in industrial machines
* Income or age in socio-economic applications
* Number of reviews in online rating systems

In this case:

We can first apply any *density estimation* approach

* The discrete attribute/class case is the same (we just use a histogram)

Then, it's a good idea to apply some *clipping*, i.e. $p_i = \max(l, \min(u, f(x_i, y_i)))$

- Densities can be very high/low, causing numerical instability

Removing Sampling Bias due to External Attributes

It is possible to remove sampling bias due to an "external" process

Consider an organ transplant program

- Candidate recipients are described by attribute x_i and wait in a queue
- ...from which they may be selected ($y_i = 1$) or not ($y_i = 0$) for surgery
- ...Surgey may then have a positive ($z_i = 1$) or negative ($z_i = 0$) outcome

Say we want to improve the outcome estimation using ML

...And possibly use to adjust the selection criterion

- The historical data will be *subject to bias* due to existing criteria
- ...But if we can estimate the *current selection proabability* $P(Y \mid X)$
- ...We can can use it as p_i for mitigating the bias!

Any classifier with probabilistic output can be used on this purpose

Sample-specific Variance

With an *MSE loss*, sample weights have also an alternative interpretation

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

$$\underset{\theta}{\operatorname{argmin}} - \sum_{i=1}^{m} \log k \exp\left(-\frac{1}{2}(y_i - h_\theta(x_i))^2\right)$$

- 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:

$$\underset{\theta}{\operatorname{argmin}} - \sum_{i=1}^{m} \frac{1}{\sigma_i^2} \log k \exp\left(-\frac{1}{2}(y_i - h_\theta(x_i))^2\right)$$

Sample-specific Variance

Which can be rewritten as:

$$
\underset{\theta}{\operatorname{argmin}} - \sum_{i=1}^m \log k \exp\left(-\frac{1}{2}\left(\frac{y_i - h_\theta(x_i)}{\sigma_i}\right)^2\right)
$$

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

This gives us a way to account for *non-uniform measurement errors*

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

The result is analogous to using a separate variance model

Stochastic Differentiation in Reinforcement Learning

Importance sampling finds applications also in *Reinforcement Learning*

While the goal of *statistical ML* is usually maximize a likelihood, e.g.:

$$
\underset{\theta}{\operatorname{argmax}}\, \mathbb{E}_{x,y \sim P}\left[f_\theta(y \mid x)\right]
$$

...The goal of RL is to *learn how to optimize* a reward, e.g.:

$$
\underset{\theta}{\operatorname{argmax}}\, \mathbb{E}_{x \sim P}\left[f(x, \pi_\theta(x))\right]
$$

Where the presented formulation focuses on *a single step* (for simplicity)

- x represents an observable *state*
- $\pi_\theta : x \mapsto a$ is a parameterized policy outputing an *action*
- $f : x, a \mapsto r$ is a *reward function*

Stochastic Differentiation in Reinforcement Learning

In tipical RL settings, the reward function is *non-differentiable*

- In AlphaGo Zero, the ultimate reward is winning a game of Go
- For OpenAI Five the goal is winning a game of Dota 2
- In this research the goal is for a robot not to fall

If we still want to use a gradient method, we need to overcome this issue

- One way is approximating f via a *differentiable critic* (e.g. a NN)
- ...Another is using a *stochastic policy*

In the latter case, π_θ defines a probability distribution $\pi_\theta(a \mid x)$

- Given a state x, we might obtain different actions a
- ...Usually according to a Normal distribution (with fixed σ)

Stochastic Differentiation in Reinforcement Learning

With a stochastic policy, the training problem becomes:

$$\operatorname*{argmax}_\theta \mathbb{E}_{x \sim P, a \sim \pi_\theta(a|x)} \left[f(x, a) \right]$$

- The semantic is not the same as the original, but the goal is similar
- The problem contains now a *double expectation*

We could try to use a Monte Carlo approach with both

- There are well established techniques for sampling x
- ...And we could sample actions $\{a_k\}_{k=1}^m$ directly from $\pi_\theta(a \mid x)$, obtaining:

$$\mathbb{E}_{a \sim \pi_\theta(a|x)} \left[f(x, a) \right] \simeq \frac{1}{m} \sum_{k=1}^m f(x, a_k)$$

...But unfortunately this expression is again non-differentiable

Stochastic Differentiation in Reinforcement Learning

It is possible to circumvent the issue via importance sampling

We sample the actions *uniformly at random*, but then we alter their distribution

- All p_i are identical, due to the uniform assumption
- The p_i^* are given by the policy itself, leading to:

$$\mathbb{E}_{a \sim \pi_\theta(a|x)} \left[f(x, a) \right] \simeq \frac{1}{m} \sum_{k=1}^m \pi_\theta(a_k \mid x) f(x, a_k)$$

- While the $f(x, a_k)$ is still just a constant
- ...The probability $\pi_\theta(a_k \mid x)$ is now *differentiable in θ*

Intuitively: we train to increase the probability of good actions

Stochastic Differentiation in Reinforcement Learning

This differentiation trick via importance sampling is a bit crude

- Uniform sampling might generate actions with very low probability
- ...Leading to noisy estimates and numerical issues

In practice, it's not a good idea to use it direcly

...But it is the basis for some famous RL methods!

- It is used to derive the original REINFORCE algorithm
- It is central to the TRPO method
- ...And to the state-of-the-art Proximal Policy Optimization method