

# Machine Learning for Anomaly Detection

**MLE SCHOOL'22**

*Machine Learning in Engineering Summer School @ TUHH*

Antonin Sulc

Hamburg, September 13, 2022

**CDCS**

CENTER FOR DATA AND COMPUTING  
IN NATURAL SCIENCES



**TUHH**  
*Technische Universität Hamburg*



Universität Hamburg  
DER FORSCHUNG | DER LEHRE | DER BILDUNG

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- > a person or thing that is different from what is usual, or not in agreement with something else and therefore not satisfactory [Cambridge Dictionary]

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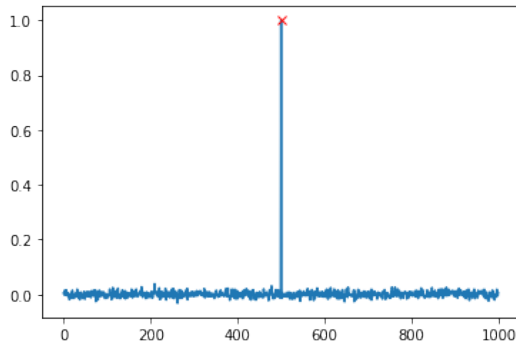
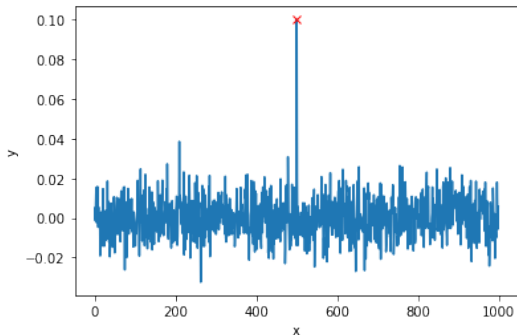
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- > something different, abnormal, peculiar, or not easily classified [Merram-Webster]

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- > something different, abnormal, peculiar, or not easily classified [Merram-Webster]
- > ...
- > A person with no perceptible faults, who consistently fails at achieving matches thru all forms of social media [Urban Dictionary]

# Point Anomaly

a single data sample that can be considered anomalous compared to the rest of the data [Wittkopp et al.(2022)Wittkopp, Wiesner, Scheinert, and Kao]



# Point Anomaly - Cont'd



EUROPE ECONOMY

## **Euro zone inflation hits another record of 9.1% as food and energy prices soar**

# Point Anomaly - Cont'd



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... Eurozone inflation hit a new record high in August of 9.1%, according to flash figures from Europe's statistics office Eurostat, with high energy prices the main driving force. **Werknghwrjhb werbn re4rhn**. The rate was above expectations, with a Reuters poll of economists anticipating a rate of 9%... [Ward-Glenton(2022)]



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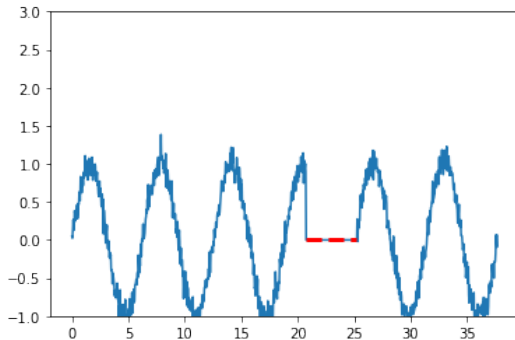
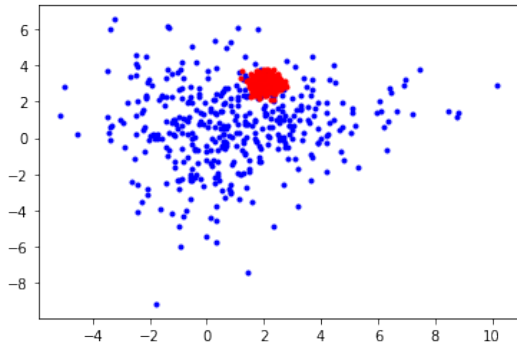
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# Group Anomaly

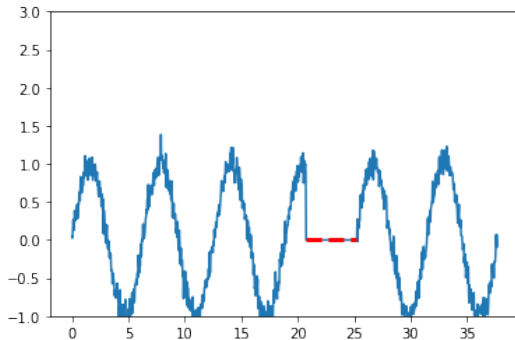
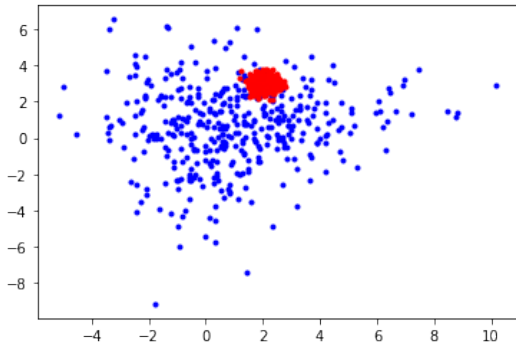
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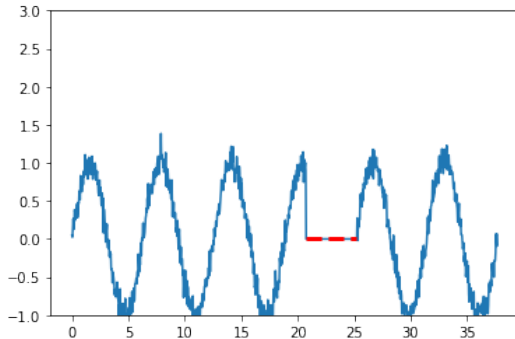
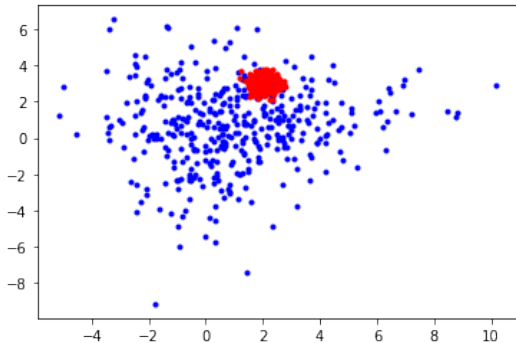
> individual samples are often not interesting,



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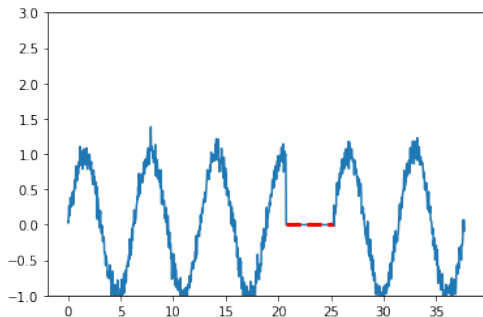
a multiple data samples that can be considered anomalous compared to the rest of the data

- > individual samples are often not interesting,
- > anomalous group of signals is an noticeably dense with respect to entire dataset.



# Contextual Anomaly

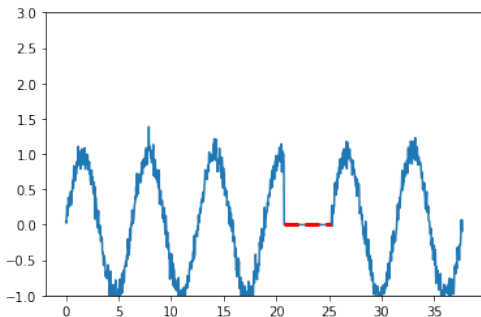
samples that are anomalous in a specific context only (but not otherwise) are called **contextual anomalies** [Wittkopp et al.(2022)Wittkopp, Wiesner, Scheinert, and Kao]



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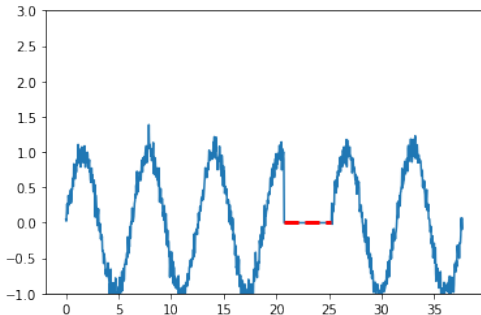
> can have the same feature-set (behavioral properties) as normal samples,



# Contextual Anomaly

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- > can have the same feature-set (behavioral properties) as normal samples,
- > but are still anomalous within a specific context defined by their contextual properties.



# Contextual Anomaly - Cont'd



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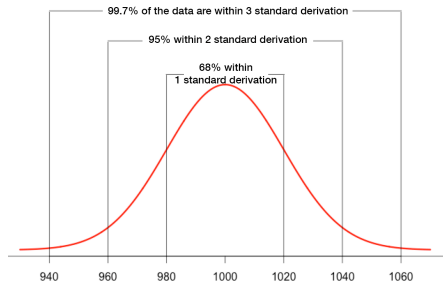


Roll your sleeves!

<https://github.com/sulcantonin/MLE2022>

# Anomaly Detection - Basics - 3-Sigma Rule

> Mean  $\mu$  defines an average value ( $\mu = 1000$ ).

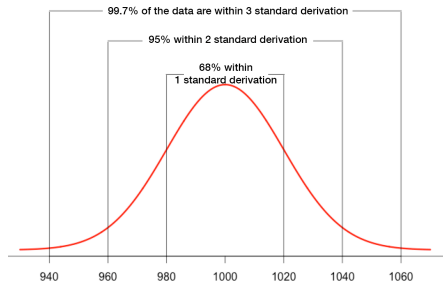


[Magakian(2018)]

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_Basics.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_Basics.ipynb)

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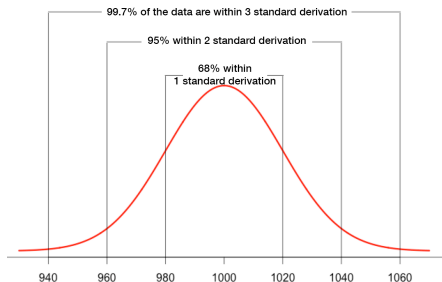


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- > 68% of all values fall between  $[\mu - \sigma, \mu + \sigma]$ , i.e. [980, 1020].

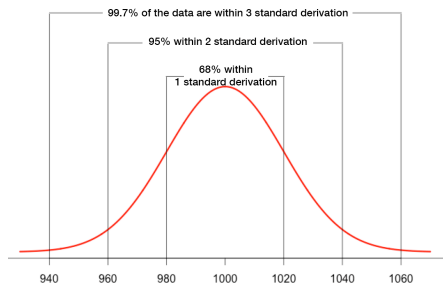


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- > 95% of all values fall between  $[\mu - 2\sigma, \mu + 2\sigma]$ , i.e. [960, 1040].

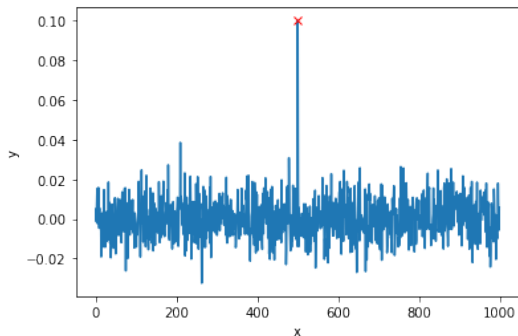


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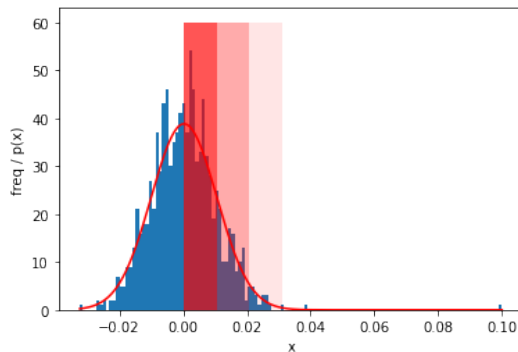
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# Anomaly Detection - 3-Sigma Example

Plot



Histogram

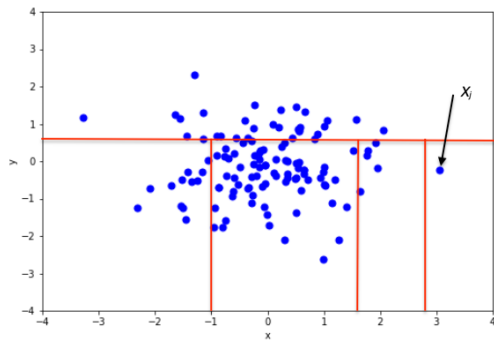
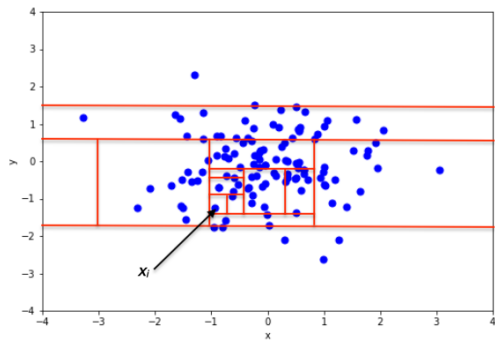


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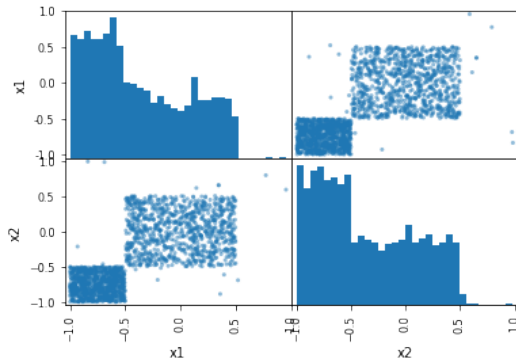
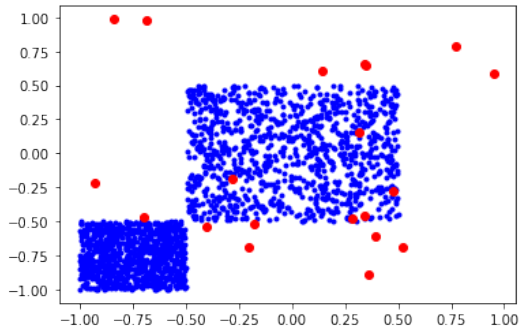
# Anomaly Detection - Isolation Forest

Isolation forest split the data space using lines that are orthogonal to the origin, and assigns higher anomaly scores to data points that need few splits to be isolated. [wik(2022)]

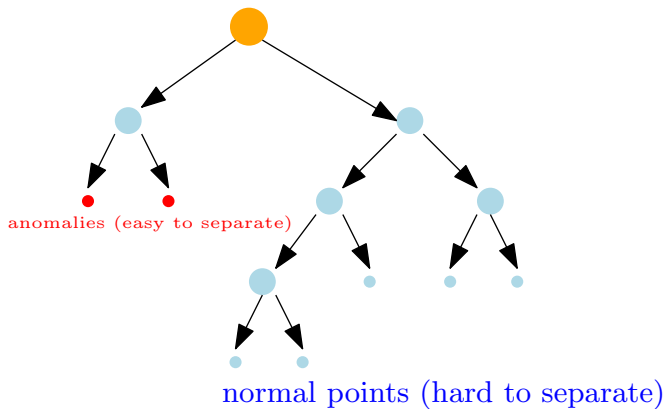


## Anomaly Detection - Isolation Forest

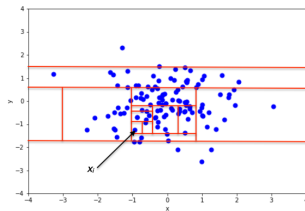
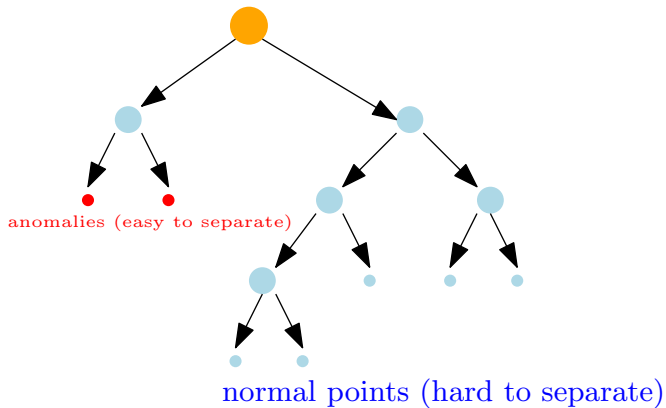
## What if the points are not normally distributed?



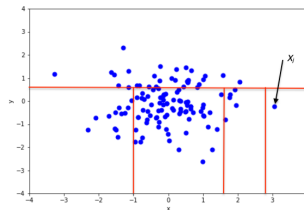
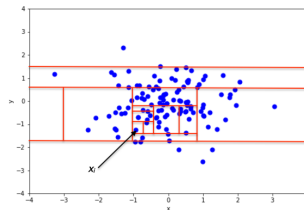
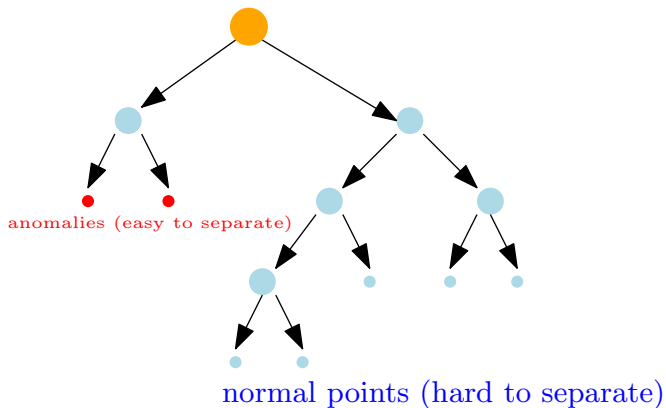
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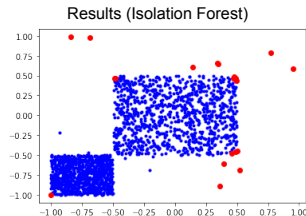
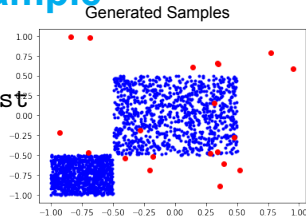
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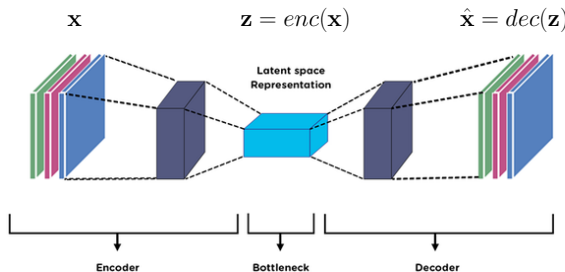
```
from sklearn.ensemble import IsolationForest
import numpy.random as r
r.seed(42)
Xn1 = r.rand(1000,2) - 0.5
Xn2 = (r.rand(1000,2) - 2) * 0.5
Xn = np.concatenate((Xn1,Xn2))
Xa = 2 * (r.rand(20,2) - 0.5)
X = np.concatenate((Xn,Xa))

cont= 20.0 / 2020.0 # ratio of anomalies
if = IsolationForest(contamination = cont, random_state = 42)
l = if.fit_predict(X)
```



# Anomaly Detection - Auto-encoder

What if we have data and want to train a model of a set of data points  $\{x_1 \dots x_N\}$ ?



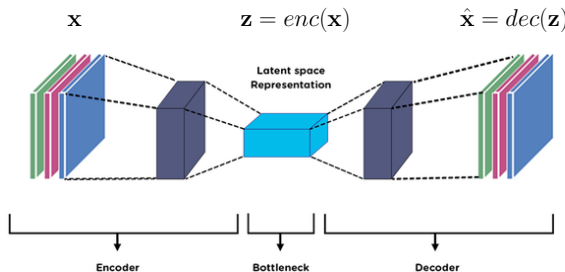
[Birla(2019)]

$$s = \|\mathbf{x} - dec(enc(\mathbf{x}))\|_2$$

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_Autoenc.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_Autoenc.ipynb)

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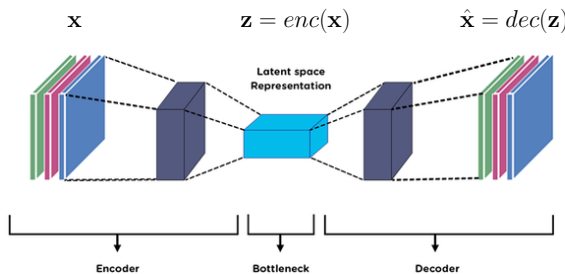
+/- Trains the network "generatively".

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+/- Trains the network "generatively".

- Technically you are not training anomaly detection, but training a model of data

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_Autoenc.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_Autoenc.ipynb)

# Anomaly Detection - Auto-encoder Example

```
enc = nn.Sequential(  
    nn.Linear(2, 8),  
    nn.ReLU(),  
    nn.Linear(8, 16))  
dec = nn.Sequential(  
    nn.Linear(16, 8),  
    nn.ReLU(),  
    nn.Linear(8, 2))  
  
def score_reconstruction(x):  
    return vector_norm(dec(enc(x)) - x, dim=-1)
```

Reconstr. loss - score

$\downarrow \|\mathbf{x} - dec(enc(\mathbf{x}))\|_2$

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_Autoenc.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_Autoenc.ipynb)

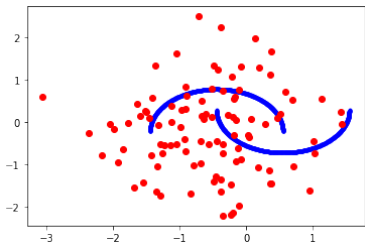
## Anomaly Detection - Auto-encoder Example Cont'd

```
optimizer = optim.Adam( list(enc.parameters()) +  
                        list(dec.parameters()))  
  
# reconstruction (X_hat)  
X_hat = model(X)  
# criterion ||X - X_hat||_2  
loss = F.mse_loss(X_hat, X)  
optimizer.zero_grad()  
loss.backward()  
optimizer.step()
```

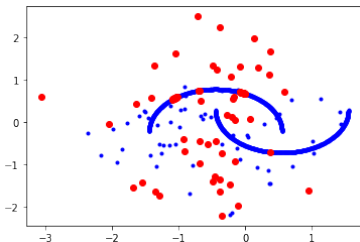
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# Anomaly Detection - Auto-encoder Example Cont'd

Input Points

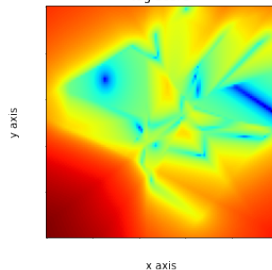


Trained Classification



$$s = \|\mathbf{x} - \text{dec}(\text{enc}(\mathbf{x}))\|_2$$

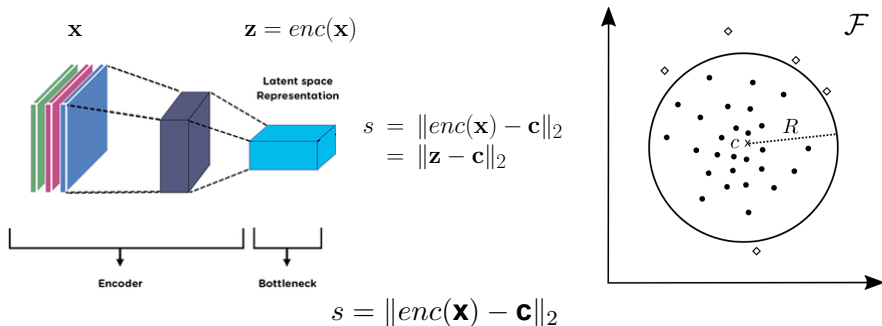
log score



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# Anomaly Detection - One Class Loss (OCL)

What if we have data and want to train a model of a set of data points  $\{x_1 \dots x_N\}$ ?



Networks train to project  $\mathbf{x}$  to fit the hypersphere center  $\mathbf{c}$

[Ruff(2019)]

- + Trains the network "discriminatively",
- One has to be careful with trivial solutions
  - i. e.  $\mathbf{c} \neq 0$ , no biases and unbounded non-linearity

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_OCL.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_OCL.ipynb)

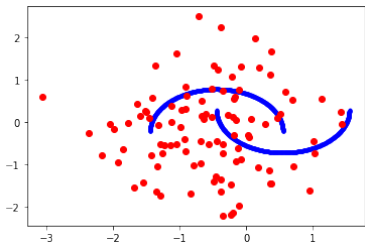
## Anomaly Detection - One Class Loss

```
enc = nn.Sequential(nn.Linear(2,8, bias = False),
                    nn.Linear(8,16, bias = False),
                    nn.Linear(16,4, bias = False))
# random center of 4D hypersphere
c = torch.randn((1,4), requires_grad = False)
optimizer = optim.Adam(enc.parameters())
# reconstruction (X_hat)
X_hat = enc(X)
loss = vector_norm(X_hat - c, dim = -1).mean()
# Optimisation enc s.t. min ||c - enc(X_hat)||_2
optimizer.zero_grad()
loss.backward()
optimizer.step()
```

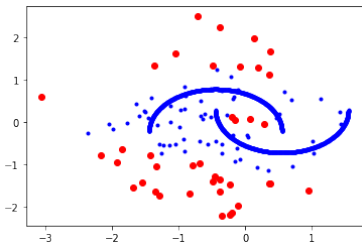
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# Anomaly Detection - One Class Loss Example Cont'd

Input Points

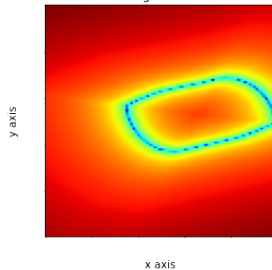


Trained Classification



$$s = \|\mathbf{c} - enc(\mathbf{x})\|_2$$

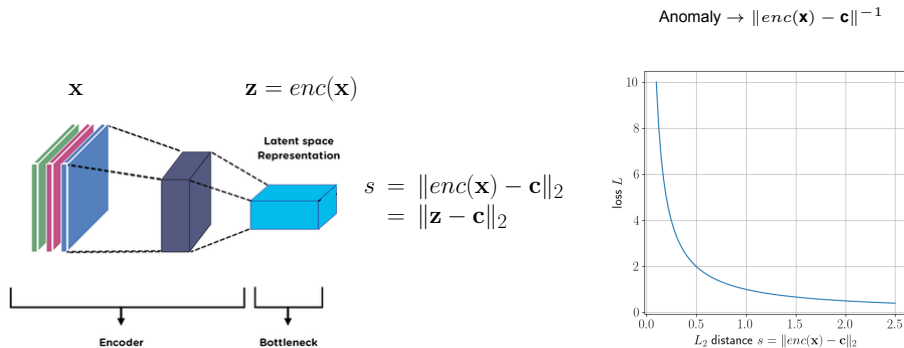
log score



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# Anomaly Detection - Semi-Supervised

What if we have data and want to train a model of a set of data points  $\{x_1 \dots x_N\}$  with very few **known** anomalies?



$$s = \|enc(\mathbf{x}) - \mathbf{c}\|^l \text{ where } l \in \{-1, 1\}$$

Known anomalies ( $l = -1$ ) encourage  $enc$  and  $\mathbf{c}$  to move away.

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_SAD.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_SAD.ipynb)



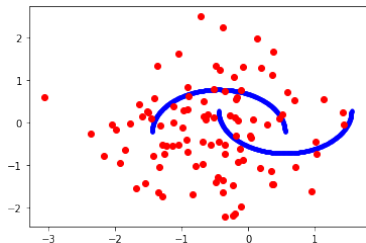
## Anomaly Detection - Semi-Supervised Example

```
enc = nn.Sequential(nn.Linear(2,8),
                    nn.Linear(8,16),
                    nn.Linear(16,4))
# random center of 4D hypersphere
enc.c = nn.Parameter(torch.randn((1,4), requires_grad = True))
optimizer = optim.Adam(enc.parameters())
# reconstruction (X_hat)
X_hat = enc(X)
loss = vector_norm((X_hat - c)**1, dim = -1).mean()
# Optimisation enc s.t. min ||c - enc(X_hat)||_2
optimizer.zero_grad()
loss.backward()
optimizer.step()
```

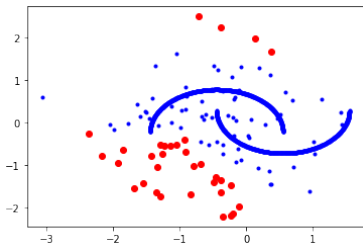
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# Anomaly Detection - Semi-supervised Example Cont'd

Input Points

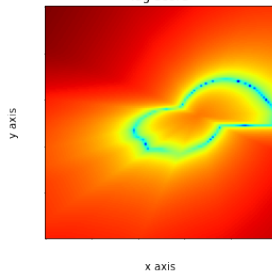


Trained Classification



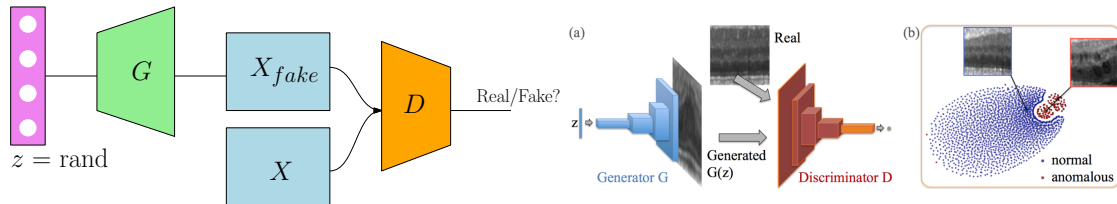
$$s = \|\mathbf{c} - enc(\mathbf{x})\|_2$$

log score



See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_SAD.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_SAD.ipynb)

# Anomaly Detection - Generative Adversarial Networks



- >  $G$  generates **fake** samples and tries to fool discriminator  $D$ .
- >  $D$  receives **fake** and **real samples** and tries to distinguish if an input is fake or real.

[Goodfellow et al.(2020)Goodfellow, Pouget-Abadie, Mirza, Xu, Warde-Farley, Ozair, Courville, and Bengio, Wiggers(2019),

Schlegl et al.(2017)Schlegl, Seeböck, Waldstein, Schmidt-Erfurth, and Langs]

$$\arg \min_{z_{\gamma}} \{ (1 - \lambda) \|x - G(z_{\gamma})\| + \lambda \text{CrossEntropyLoss}(D(G(z_{\gamma})), 1) \}$$

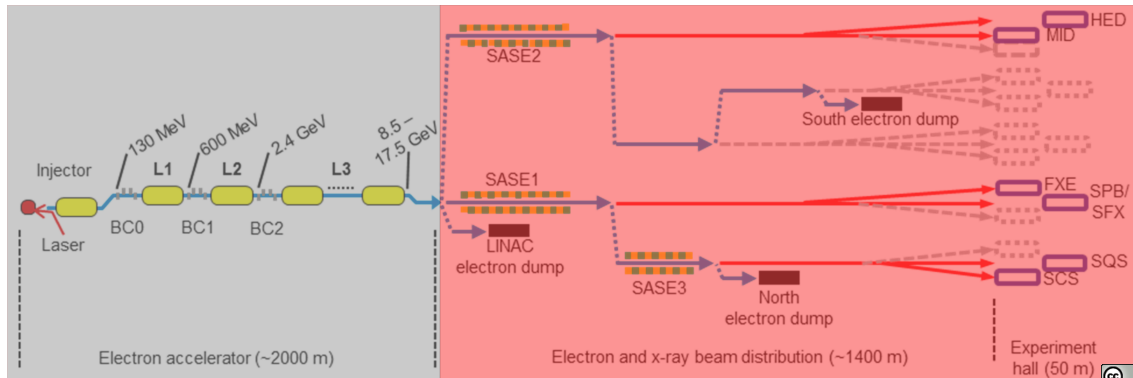
See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_GAN.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_GAN.ipynb)

# Anomaly Detection at European XFEL

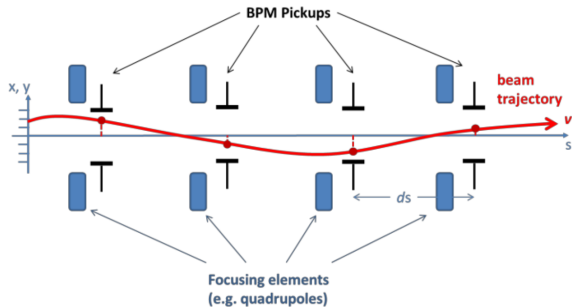
# Orbit Monitoring

## Assumption

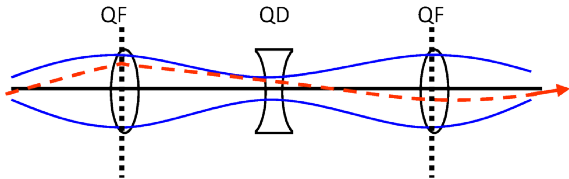
There is a systematic pattern shown in orbits given by the physical construction of EuXFEL.



# Orbit Monitoring - FODO Lattice

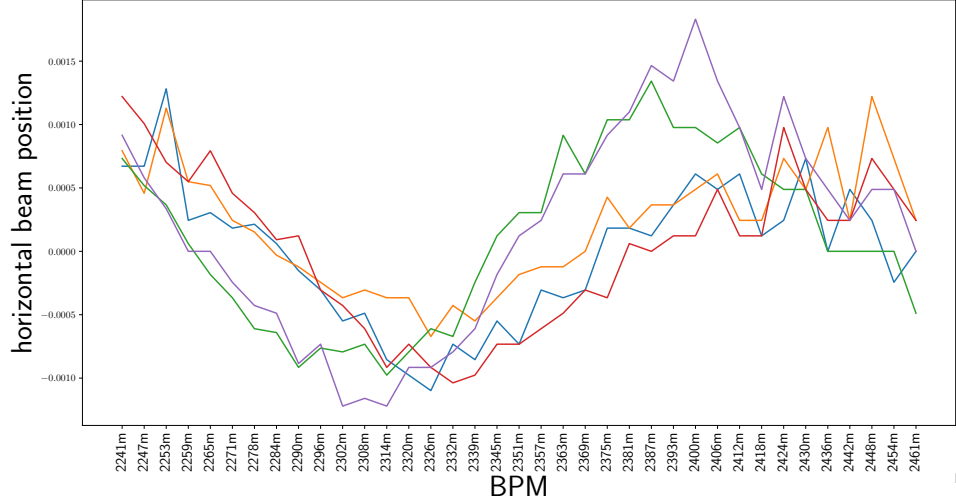


[Wendt(2011)]

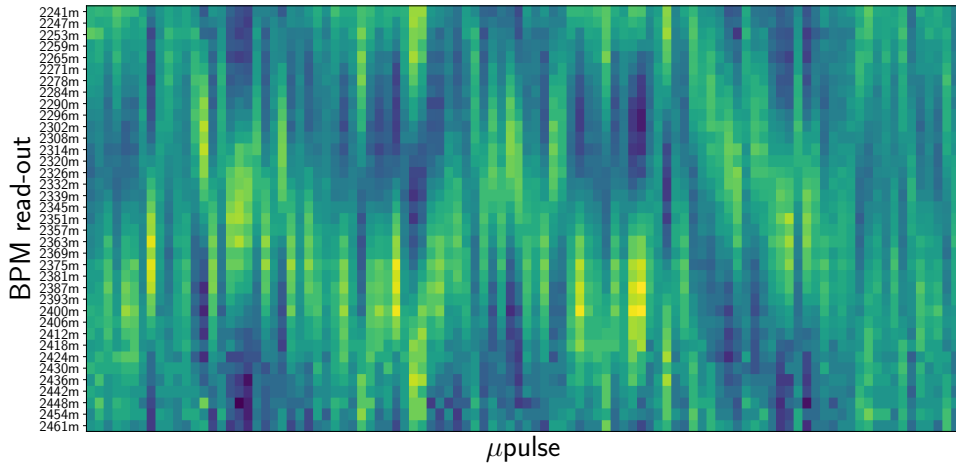


[Holzer(2006)]

# Orbit Monitoring

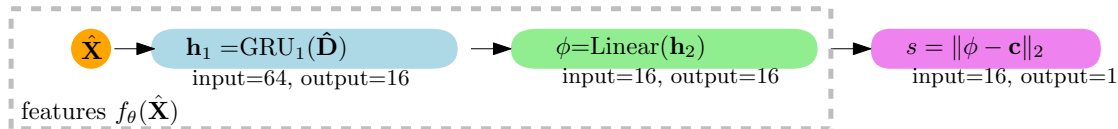


# Orbit Monitoring





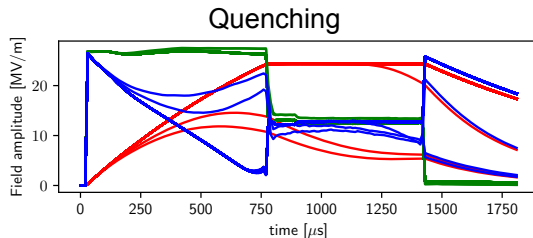
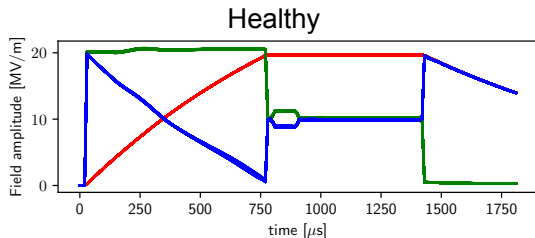
# Orbit Monitoring



```
rnn = nn.GRU(64,16)
lin = nn.Linear(16,16)
c = nn.randn((16))
s = vector_rnom(c - lin(rnn(x)[0], dim = -1)
```

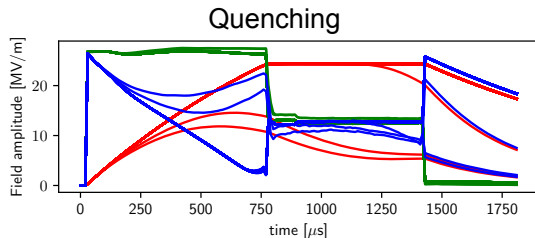
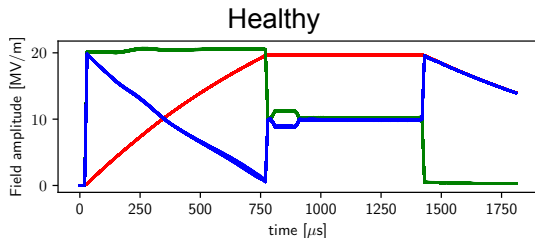
See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_orbit.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_orbit.ipynb)

# Monitoring Superconducting LLRF Cavities



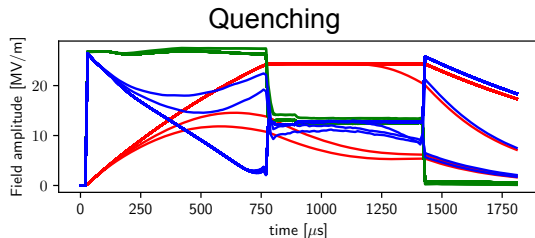
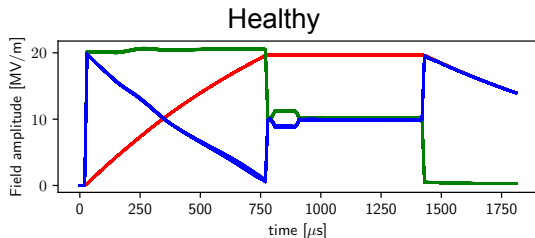
- > We record an envelope (phase, amplitude) of three signals - **probe**, **forward** and **reflected** signals.

# Monitoring Superconducting LLRF Cavities



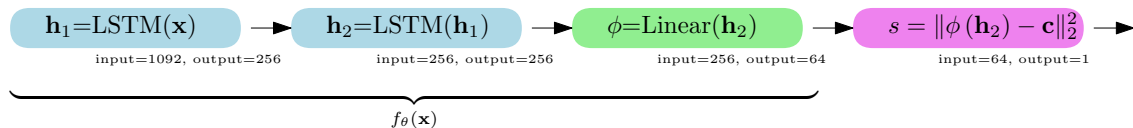
- > We record an envelope (phase, amplitude) of three signals - **probe**, **forward** and **reflected** signals.
- > Each signal consists of a pair of 1820 values (amplitude, phase) per pulse.

# Monitoring Superconducting LLRF Cavities



- > We record an envelope (phase, amplitude) of three signals - **probe**, **forward** and **reflected** signals.
- > Each signal consists of a pair of 1820 values (amplitude, phase) per pulse.
- > Quench (right) means a loss of superconductivity in a cavity, which has a significant effect on the quality factor.

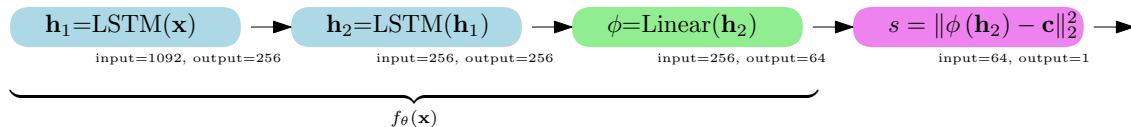
# Data-Driven Monitoring of Superconducting LLRF Cavities



- > A RNN is assigning a score to series of cavity pulses.

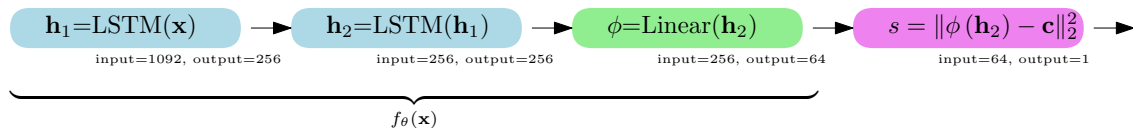
See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_cavity.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_cavity.ipynb)

# Data-Driven Monitoring of Superconducting LLRF Cavities



- > A RNN is assigning a score to series of cavity pulses.
- > Each datum  $\mathbf{x}$  (pulse) consist of (probe, forward and reflected signals).

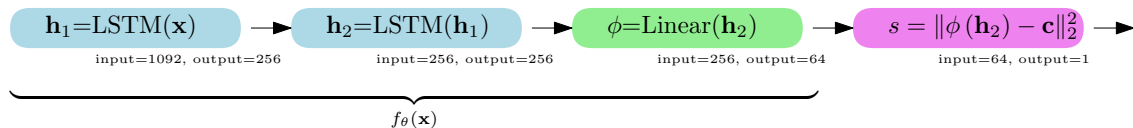
# Data-Driven Monitoring of Superconducting LLRF Cavities



- > A RNN is assigning a score to series of cavity pulses.
- > Each datum  $\mathbf{x}$  (pulse) consist of (probe, forward and reflected signals).
- > We have a disproportionately smaller dataset with faults (1300 faults) and (almost) unlimited access to healthy data.

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_cavity.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_cavity.ipynb)

# Data-Driven Monitoring of Superconducting LLRF Cavities



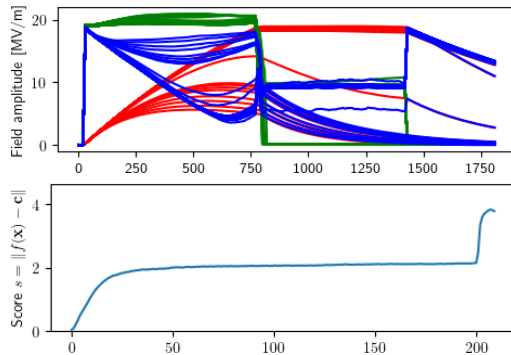
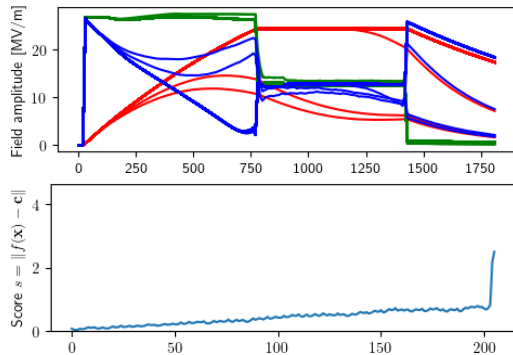
- > A RNN is assigning a score to series of cavity pulses.
- > Each datum  $\mathbf{x}$  (pulse) consist of (probe, forward and reflected signals).
- > We have a disproportionately smaller dataset with faults (1300 faults) and (almost) unlimited access to healthy data.
- > Semi-supervised anomaly loss [Ruff(2019)]

$$L(\theta) = \|f_{\theta}(\mathbf{x}) - \mathbf{c}\|_2^y + \|f_{\theta}(\mathbf{x}) - \mathbf{c}\|_2 \text{ where } y \in \{-1, 1\}.$$

See [https://github.com/sulcantonin/MLE2022/blob/main/MLE\\_cavity.ipynb](https://github.com/sulcantonin/MLE2022/blob/main/MLE_cavity.ipynb)



# Results - Quenches




# Thank you!

This is the joint work of A. Eichler and Raimund Kammering!

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[euro-zone-inflation-hits-another-record-of-9point1percent-as-food-and-en](https://www.cnn.com/2022/08/31/euro-zone-inflation-hits-another-record-of-9point1percent-as-food-and-en)  
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