

Tutorial on Anomaly Detection

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CDCS

CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES



TUHH
Technische Universität Hamburg



Universität Hamburg

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What's anomaly

- > A person with no perceptible faults, who consistently fails at achieving matches thru all forms of social media [Urban Dictionary]

What's anomaly

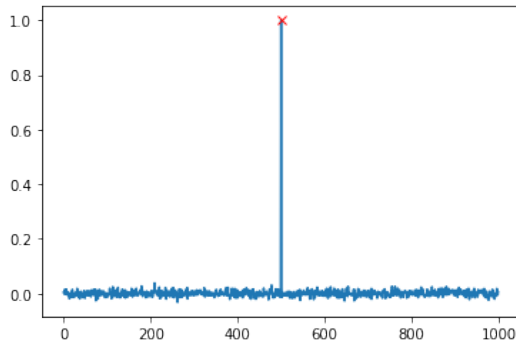
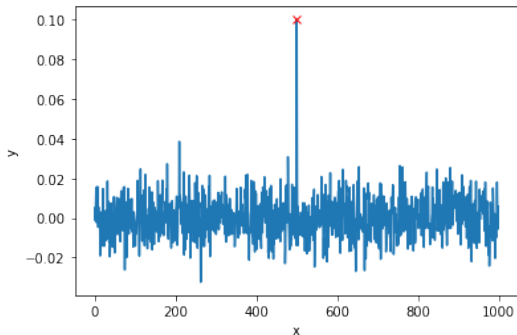
- > A person with no perceptible faults, who consistently fails at achieving matches thru all forms of social media [Urban Dictionary]
- > a person or thing that is different from what is usual, or not in agreement with something else and therefore not satisfactory [Cambridge Dictionary]

What's anomaly

- > A person with no perceptible faults, who consistently fails at achieving matches thru all forms of social media [Urban Dictionary]
- > a person or thing that is different from what is usual, or not in agreement with something else and therefore not satisfactory [Cambridge Dictionary]
- > a thing, situation, etc. that is different from what is normal or expected [Oxford 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)]

Point Anomaly - Cont'd



EUROPE ECONOMY

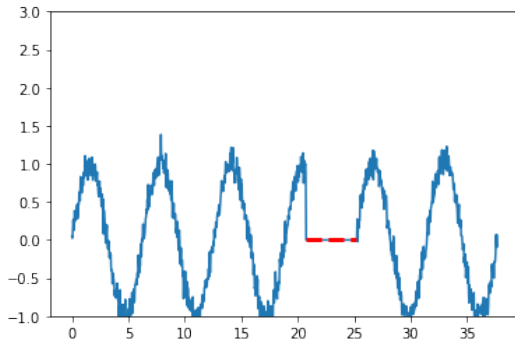
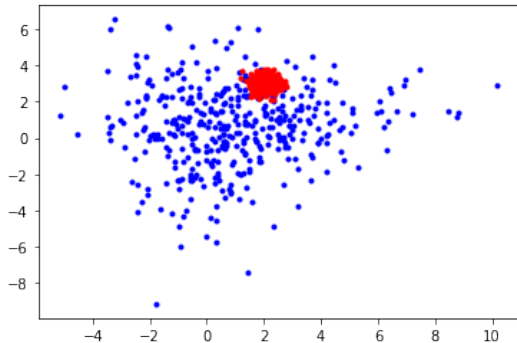
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Group Anomaly

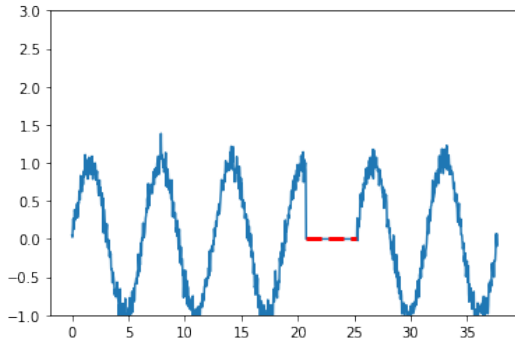
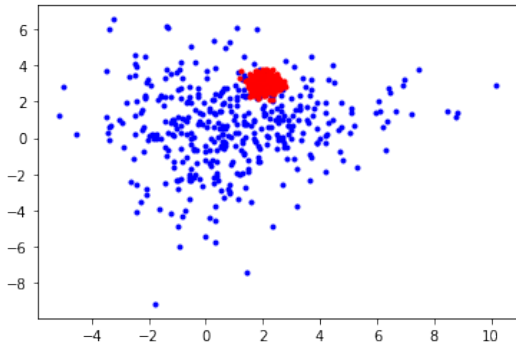
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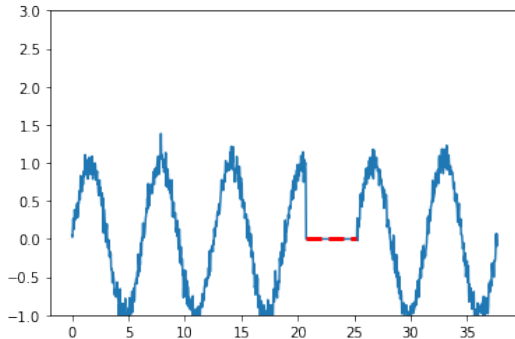
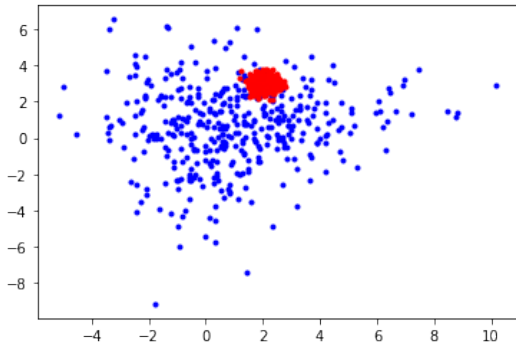
> individual samples are often not interesting,



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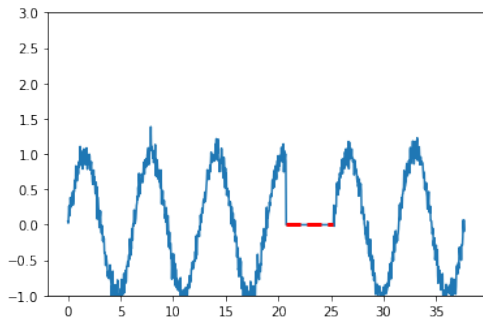
a multiple data samples that can be considered anomalous compared to the rest of the data

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



Contextual Anomaly

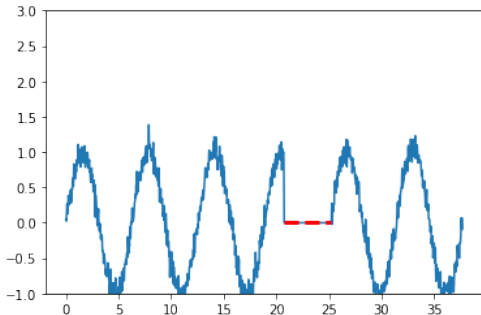
samples that are anomalous in a specific context only (but not otherwise) are called **contextual anomalies** [Wittkopp et al.(2022)Wittkopp, Wiesner, Scheinert, and Kao]



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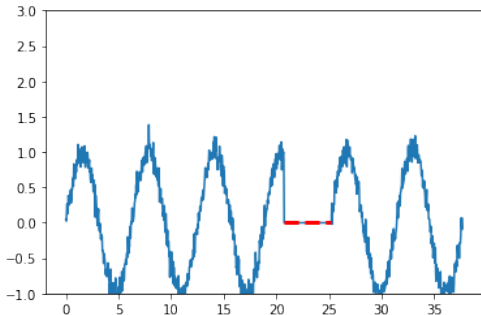
> can have the same feature-set (behavioral properties) as normal samples,



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



EUROPE ECONOMY

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Contextual 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. **We enjoyed delicious pizza with a pineapple.** The rate was above expectations, with a Reuters poll of economists anticipating ...

Contextual Anomaly - Cont'd



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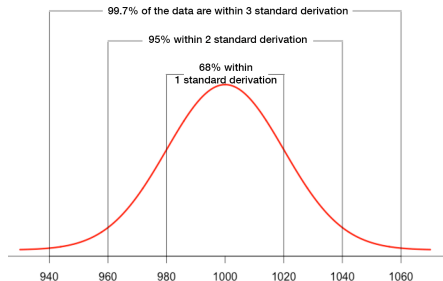


Roll your sleeves!

<https://github.com/sulcantonin/ICFA-Beam-2022>

Anomaly Detection - Basics - 3-Sigma Rule

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

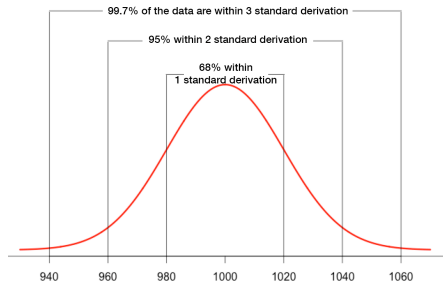


[Magakian(2018)]

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/basics.ipynb>

Anomaly Detection - Basics - 3-Sigma Rule

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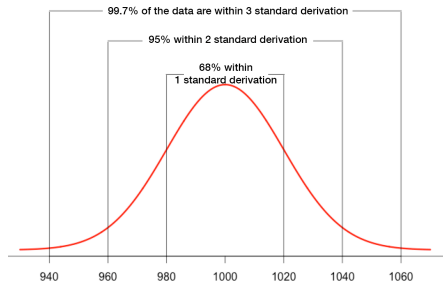


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Anomaly Detection - Basics - 3-Sigma Rule

- > Mean μ defines an average value ($\mu = 1000$).
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- > 68% of all values fall between $[\mu - \sigma, \mu + \sigma]$, i.e. [980, 1020].

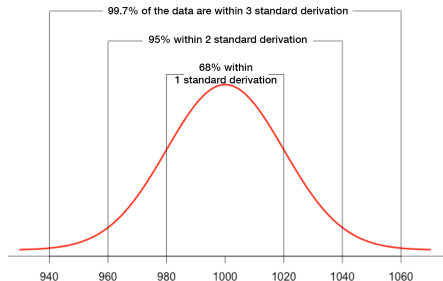


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Anomaly Detection - Basics - 3-Sigma Rule

- > Mean μ defines an average value ($\mu = 1000$).
- > Standard deviation σ , defines how far the normal distribution is spread around the mean ($\sigma = 20$).
- > 68% of all values fall between $[\mu - \sigma, \mu + \sigma]$, i.e. [980, 1020].
- > 95% of all values fall between $[\mu - 2\sigma, \mu + 2\sigma]$, i.e. [960, 1040].
- > 99.7% of all values fall between $[\mu - 3\sigma, \mu + 3\sigma]$

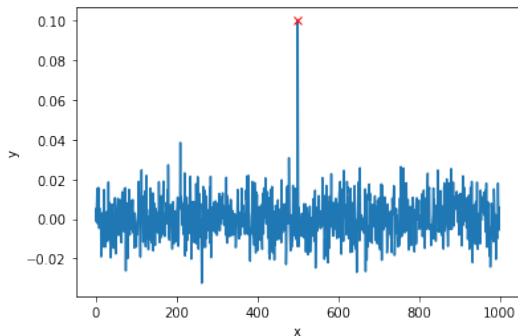


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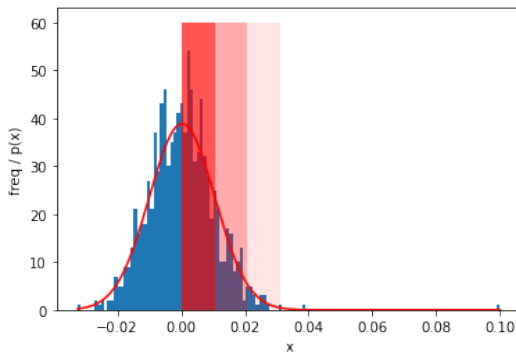
See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/basics.ipynb>

Anomaly Detection - 3-Sigma Example

Plot



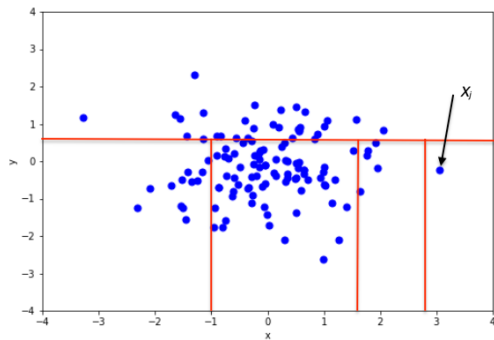
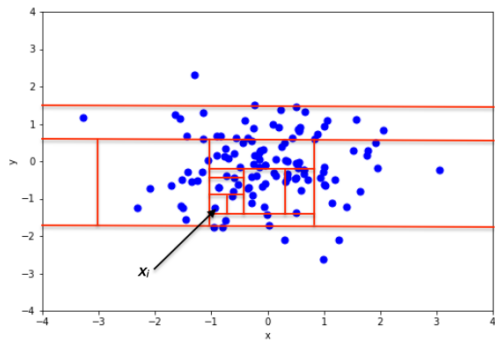
Histogram



See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/basics.ipynb>

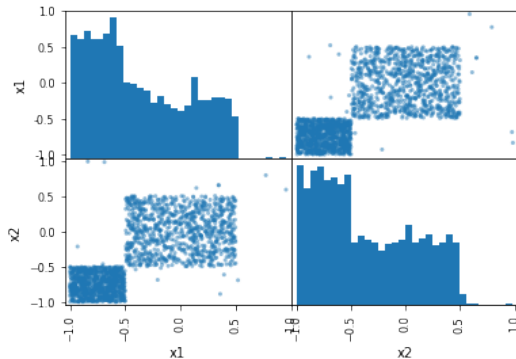
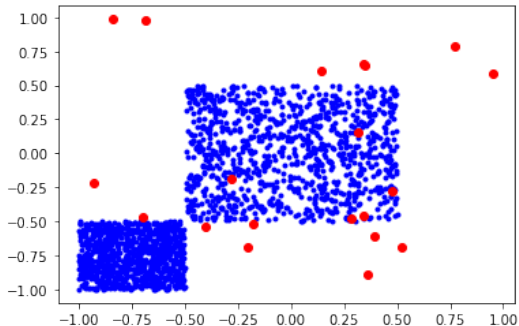
Anomaly Detection - Isolation Forest

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)]

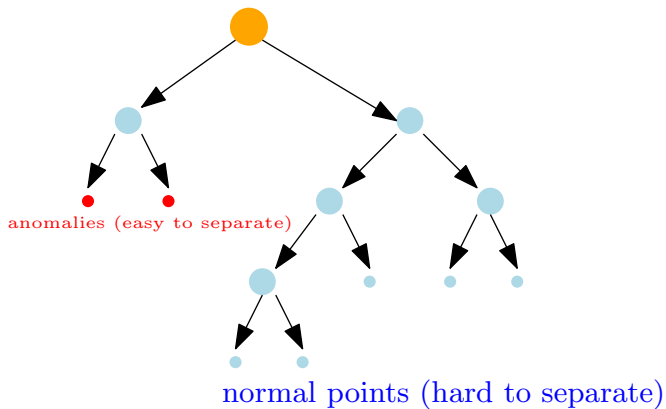


Anomaly Detection - Isolation Forest

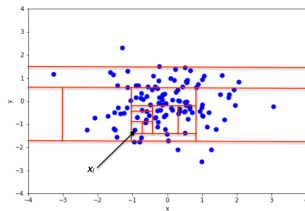
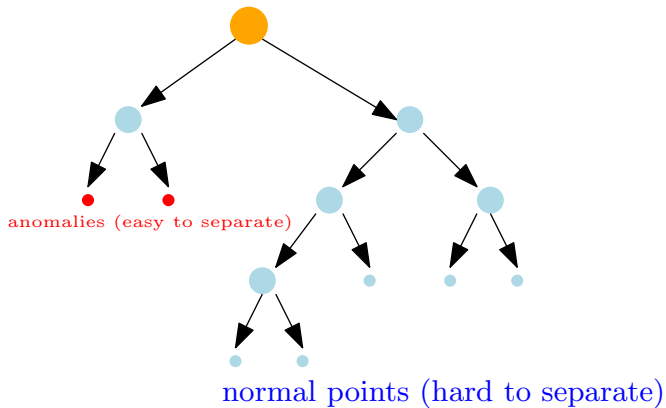
What if the points are not normally distributed?



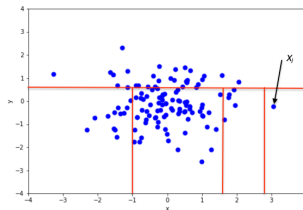
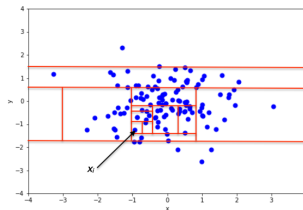
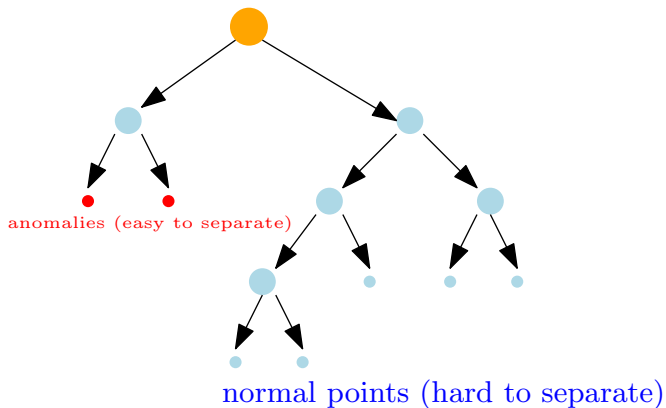
Anomaly Detection - Isolation Forest



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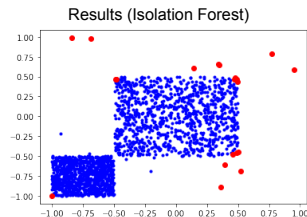
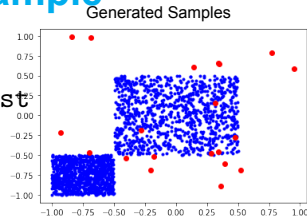


Anomaly Detection - Isolation Forest Example

```
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))
```

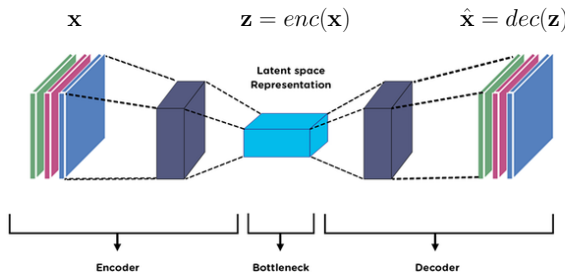
```
cont= 20.0 / 2020.0 # ratio of anomalies
```

```
f = IsolationForest(contamination = cont, random_state = 42)
l = f.fit_predict(X)
```



Anomaly Detection - Auto-encoder

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



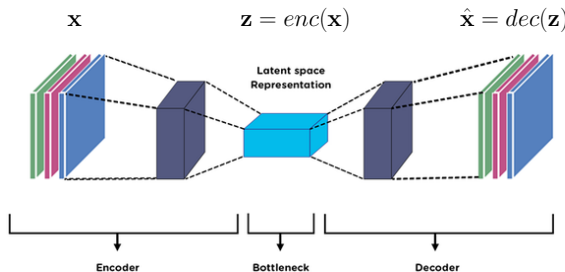
[Birla(2019)]

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

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/autoencoder.ipynb>

Anomaly Detection - Auto-encoder

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[Birla(2019)]

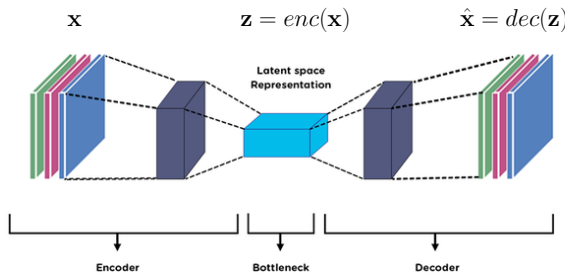
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+/- Trains the network "generatively".

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/autoencoder.ipynb>

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)]

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

+/- Trains the network "generatively".

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

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/autoencoder.ipynb>

Anomaly Detection - Auto-encoder Example

```
enc = nn.Sequential(  
    nn.Linear(2, 8),  
    nn.ReLU(),  
    nn.Linear(8, 16),  
    nn.ReLU(),  
    nn.Linear(16, 1))  
dec = nn.Sequential(  
    nn.Linear(1, 8),  
    nn.ReLU(),  
    nn.Linear(8, 16),  
    nn.ReLU(),  
    nn.Linear(16, 2))  
  
Reconstr. loss - score  
  
↓  $\|\mathbf{x} - dec(enc(\mathbf{x}))\|$   
  
def score_reconstruction(x):  
    return vector_norm(dec(enc(x)) - x, dim=-1)
```

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/autoencoder.ipynb>

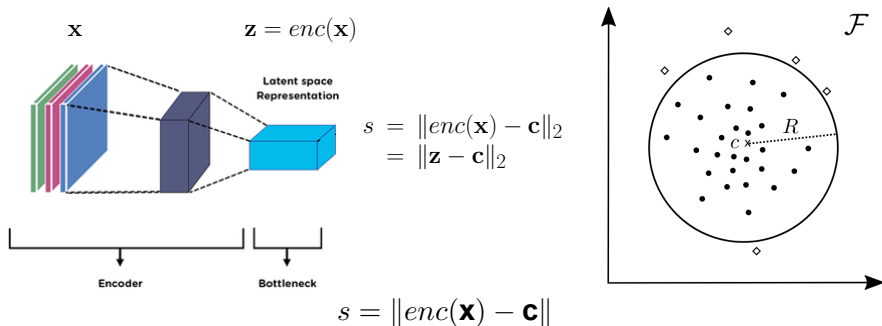
Anomaly Detection - Auto-encoder Example Cont'd

```
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()
```

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/autoencoder.ipynb>

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 trains 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/ICFA-Beam-2022/blob/main/oneclass.ipynb>

Anomaly Detection - One Class Loss

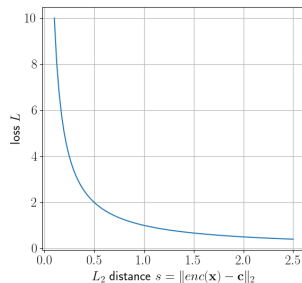
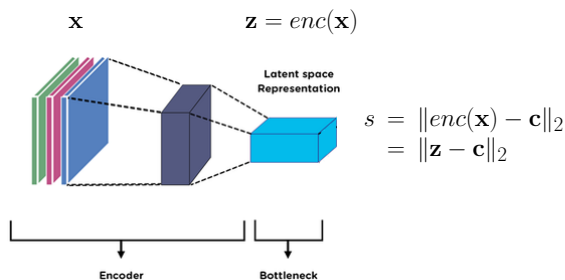
```
enc = nn.Sequential(nn.Linear(2,8, bias = False),  
                    nn.Linear(8,16, bias = False),  
                    nn.Linear(16,4, bias = False))  
# random center of 4D hypersphere  
c = torch.randn((1,4), requires_grad = False)  
optimizer = optim.Adam(enc.parameters())  
# reconstruction (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()
```

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/oneclass.ipynb>

Anomaly Detection - Semi-Supervised Anomaly Loss

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?

$$\text{Anomaly} \rightarrow \|enc(\mathbf{x}) - \mathbf{c}\|^{-1}$$



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

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

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/sal.ipynb>

Anomaly Detection - Semi-Supervised Example

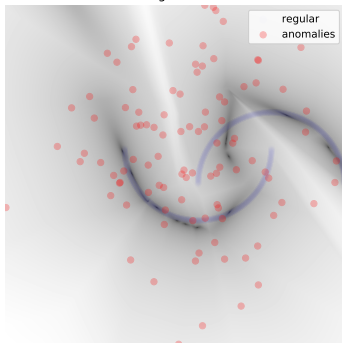
```
enc = nn.Sequential(nn.Linear(2,8),
                    nn.Linear(8,16),
                    nn.Linear(16,4))
# random center of 4D hypersphere
enc.c = nn.Parameter(torch.randn((1,4), requires_grad = True))
optimizer = optim.Adam(enc.parameters())
# reconstruction (X_hat)
X_hat = enc(X)
loss = (vector_norm((X_hat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

See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/sal.ipynb>

Comparison - Autoencoder + OCL + SAL

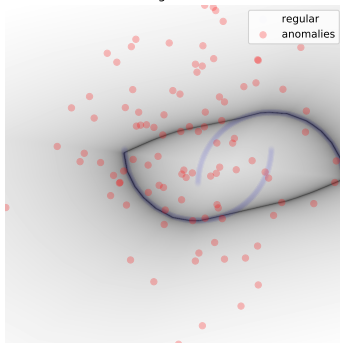
Autoencoder

log score



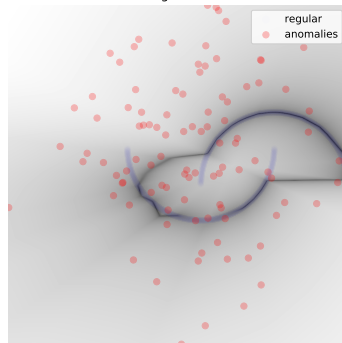
One Class Loss

log score

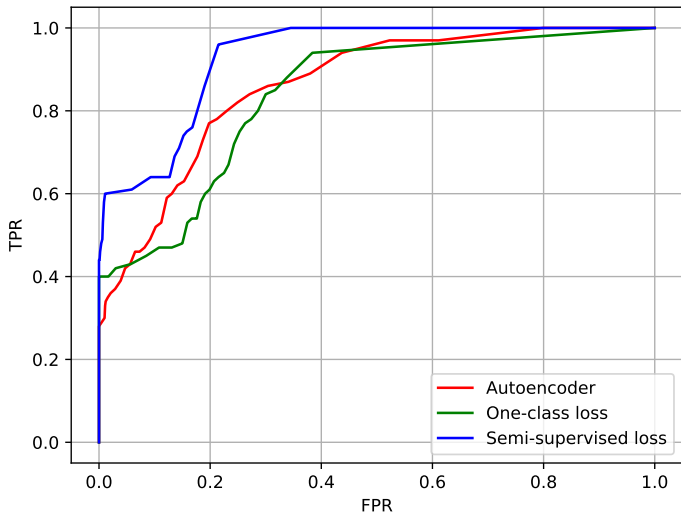


Semi-Supervised

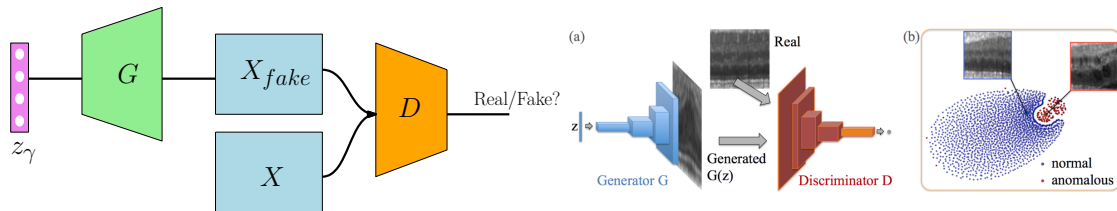
log score



Anomaly Detection - ROC Curve



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.

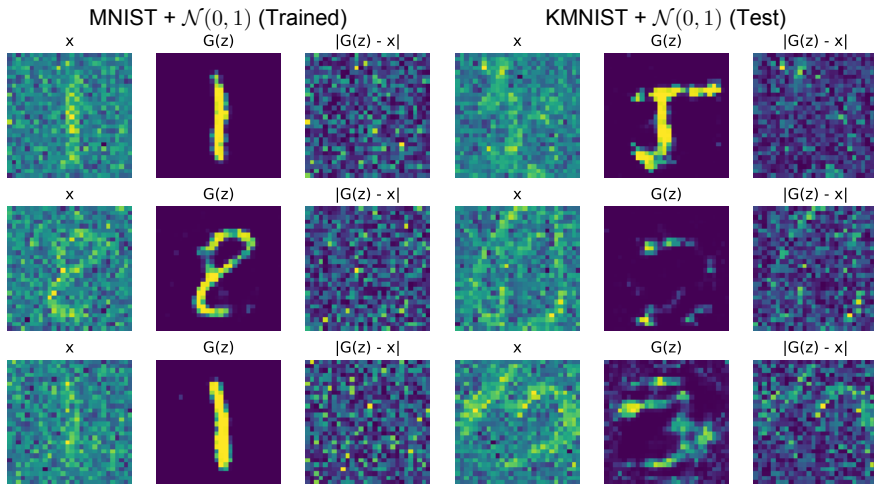
[Goodfellow et al.(2020)Goodfellow, Pouget-Abadie, Mirza, Xu, Warde-Farley, Ozair, Courville, and Bengio, Wiggers(2019),

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

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

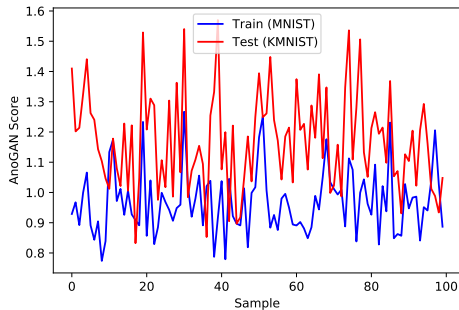
See <https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/gan.ipynb>

GAN and AnoGAN Example

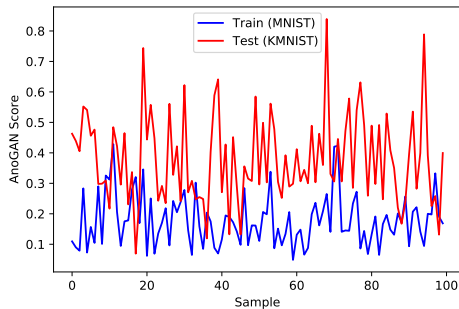


GAN and AnoGAN Example

Noisy Inputs Scores



Noise-Free Samples




Thank you!

Contact

DESY. Deutsches
Elektronen-Synchrotron

www.desy.de

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MCS DESY
antonin.sulc@desy.de

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



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