Tutorial on Anomaly Detection

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CDCS
CENTER FOR DATA AND COMPUTING IN NATURAL SCIENCES

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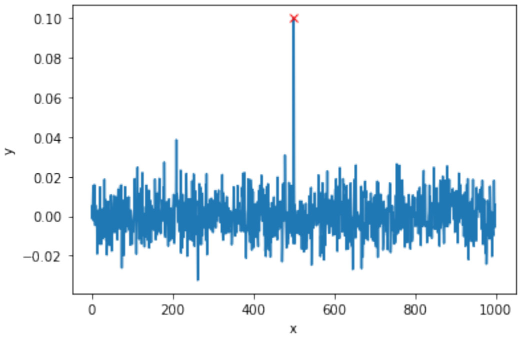
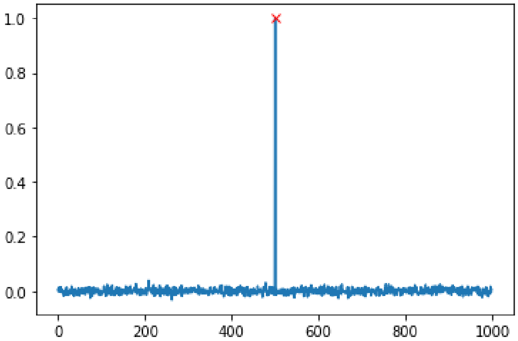
Point Anomaly

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

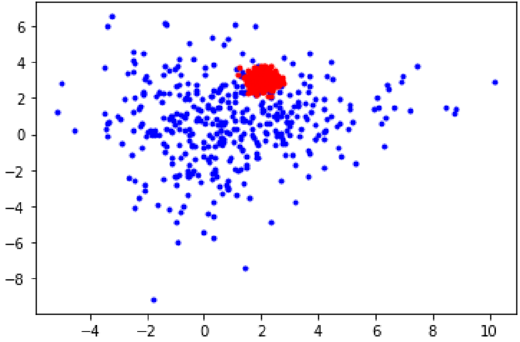
Euro zone inflation hits another record of 9.1% as food and energy prices soar

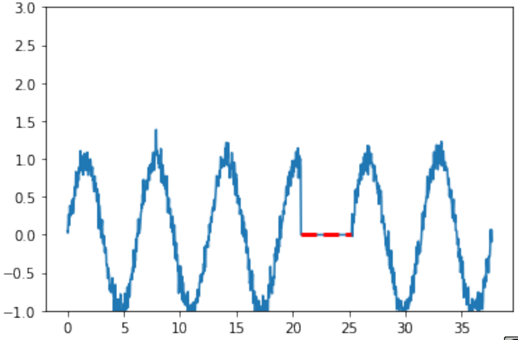
... Eurozone inflation hit a new record high in August of 9.1%, according to flash figures from Europe's statistics office Eurostat, with high energy prices the main driving force. Werknghwrjhb werbn re4rhn. The rate was above expectations, with a Reuters poll of economists anticipating a rate of 9%...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

Group Anomaly

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]

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

In context of meadows and suns

Something is wrong with sun and grass is synthetic.

In context of Teletubies

Sun still contains ”a person” but it isn’t clearly isn’t a baby.

Contextual Anomaly - Cont'd

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EUROPE ECONOMY

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

... 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. Pineapples are getting more expensive. Italians can't put them on pizza. The rate was above expectations, with a Reuters poll of economists anticipating ...

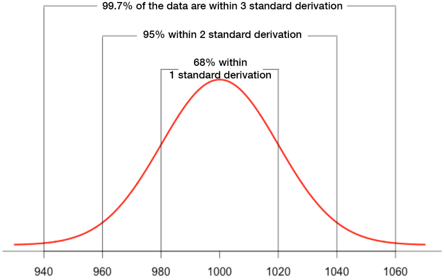
1. Talking about pineapple prices isn't relevant although it is finance relevant.
2. Pineapple does not belong to pizza!

Roll your sleeves!

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

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].



[Magakian(2018)]

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

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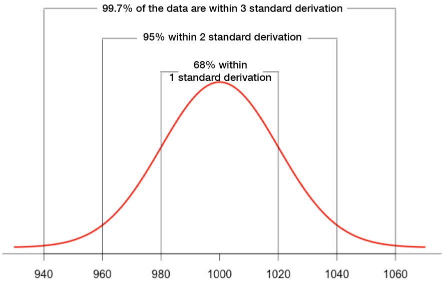

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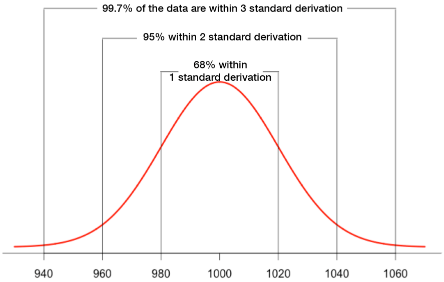

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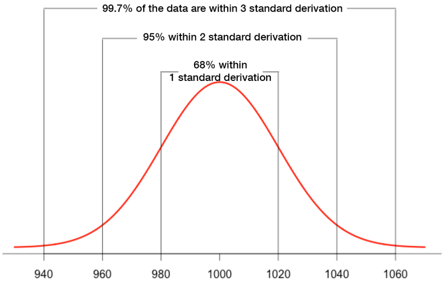
Anomaly Detection - Basics - 3-Sigma Rule

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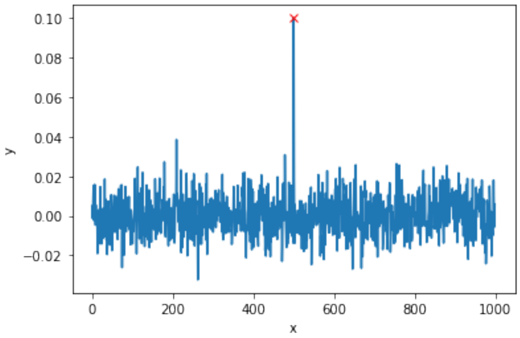
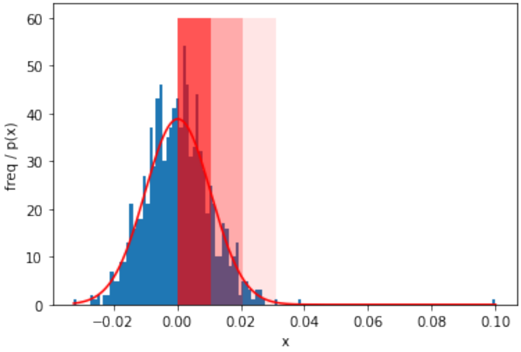
See https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/basics.ipynb

Anomaly Detection - 3-Sigma Example

Plot



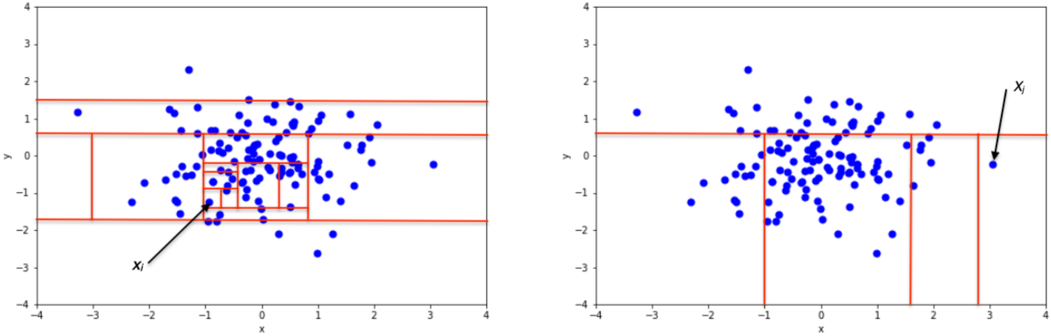
Histogram



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

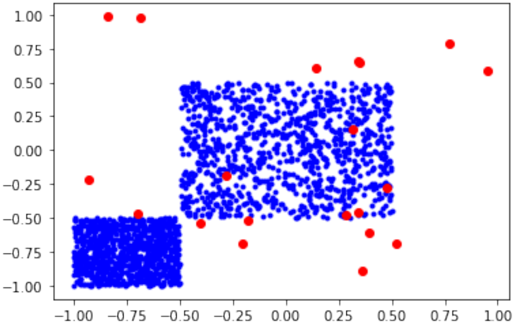
Anomaly Detection - Isolation Forest

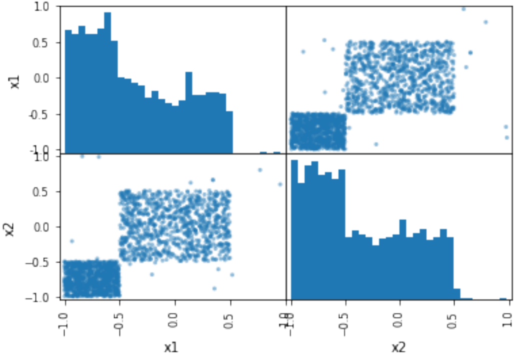
Isolation forest split the data space using lines that are orthogonal to the origin, and assigns higher anomaly scores to data points that need few splits to be isolated. [wik(2022)]



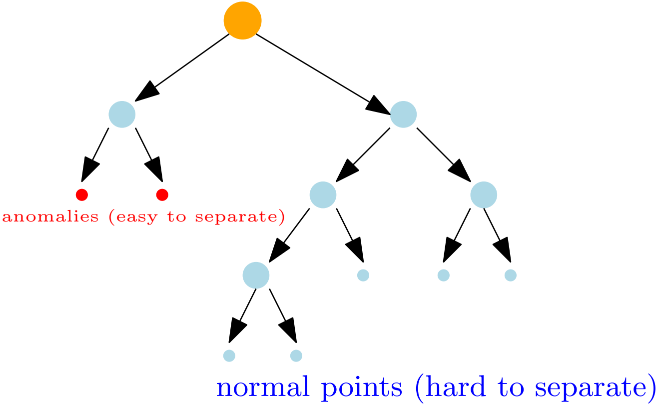
Anomaly Detection - Isolation Forest

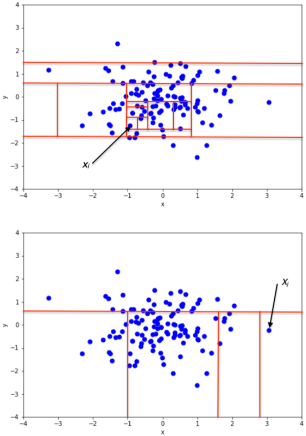
What if the points are not normally distributed?





Anomaly Detection - Isolation Forest



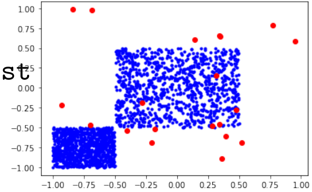


Anomaly Detection - Isolation Forest Example

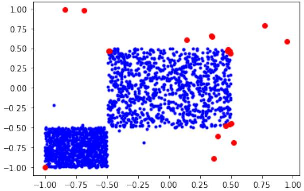
```python
from sklearn.ensemble import IsolationForest
import numpy.random as r
r.seed(42)
Xn1 = r.rand(1000,2) - 0.5
Xn2 = (r.rand(1000,2) - 2) * 0.5
Xn = np.concatenate((Xn1,Xn2))
Xa = 2 * (r.rand(20,2) - 0.5)
X = np.concatenate((Xn,Xa))

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

Generated Samples



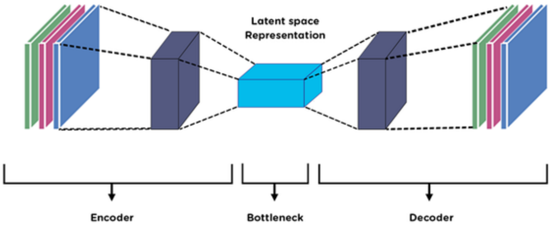
Results (Isolation Forest)



Anomaly Detection - Auto-encoder

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

$\mathbf{x}$ $\mathbf{z} = enc(\mathbf{x})$ $\hat{\mathbf{x}} = dec(\mathbf{z})$



[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))
def score_reconstruction(x):
    return vector_norm(dec(enc(x)) - x, dim=-1)
```

Reconstr. loss - score

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

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

Anomaly Detection - Auto-encoder Example Cont'd

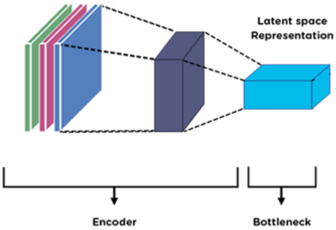
```
optimizer = optim.Adam( list(enc.parameters()) +
                        list(dec.parameters()))
# reconstruction (X_hat)
X_hat = model(X)
# criterion ||X - X_hat||_2
loss = F.mse_loss(X_hat, X)
optimizer.zero_grad()
loss.backward()
optimizer.step()
```

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

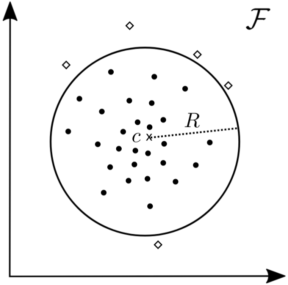
Anomaly Detection - One Class Loss (OCL)

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

$\mathbf{x}$ $\qquad\qquad\qquad$ $\mathbf{z} = enc(\mathbf{x})$



$$
\begin{aligned}
s &= \|enc(\mathbf{x}) - \mathbf{c}\|_2 \\
&= \|\mathbf{z} - \mathbf{c}\|_2
\end{aligned}
$$



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

Networks trains to project **x** to fit the hyphersphere center **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()
```

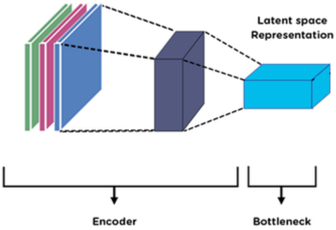
See https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/oneclass.ipynb

Anomaly Detection - Semi-Supervised Anomaly Loss (SAL)

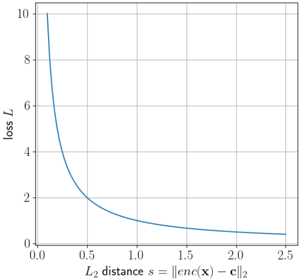
What if we have data and want to train a model of a set of data points $\{x_1 \dots x_N\}$ with very few **known** anomalies?

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

$\mathbf{x}$ $\qquad$ $\mathbf{z} = enc(\mathbf{x})$



$$
\begin{aligned}
s &= \|enc(\mathbf{x}) - \mathbf{c}\|_2 \\
  &= \|\mathbf{z} - \mathbf{c}\|_2
\end{aligned}
$$



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

- Known anomalies ($l = -1$) encourage enc and **c** to move away.
- Unlike classification loss, SAL minimizes entropy of normal samples and maximizes entropy of anomalies.

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

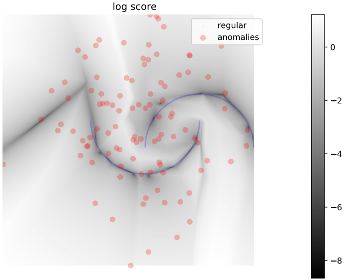
Anomaly Detection - Semi-Supervised Example

```
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()
```

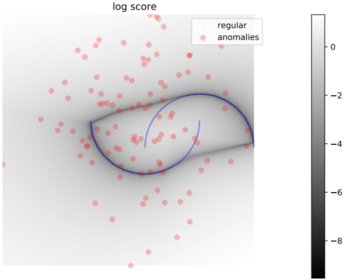
See https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/sal.ipynb

Comparison - Autoencoder + OCL + SAL

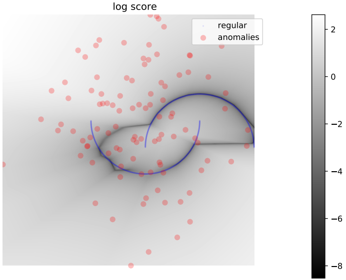
Autoencoder



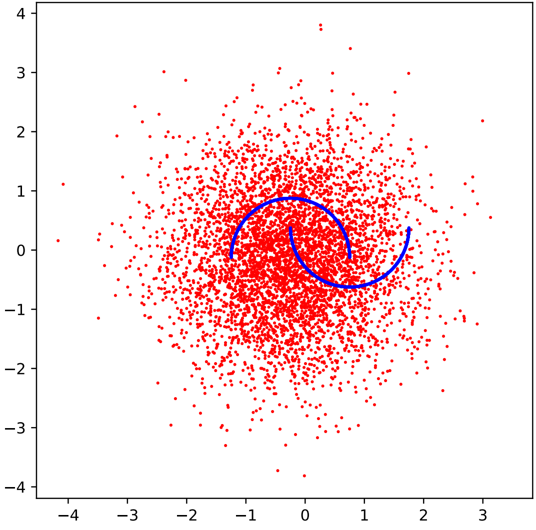
One Class Loss

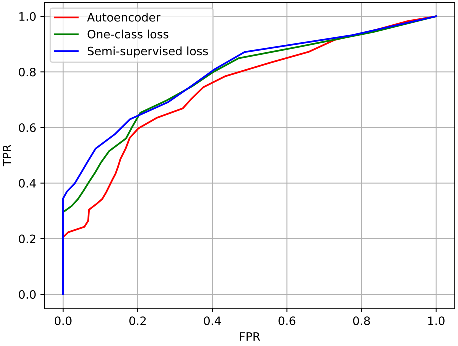


Semi-Supervised

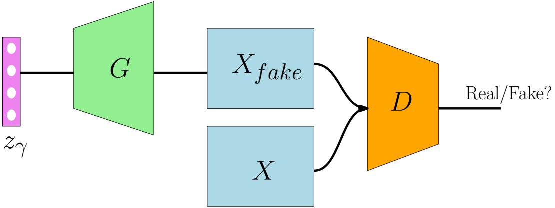


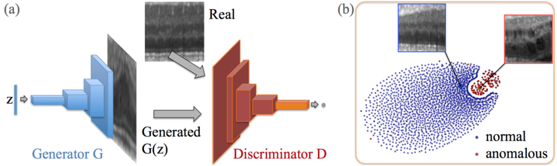
Anomaly Detection - ROC Curve





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.

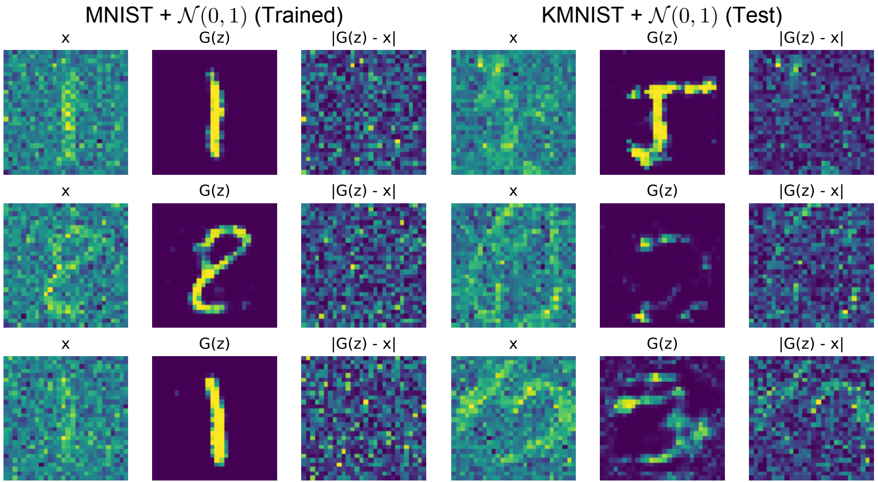
[Goodfellow et al.(2020)Goodfellow, Pouget-Abadie, Mirza, Xu, Warde-Farley, Ozair, Courville, and Bengio, Wiggers(2019),

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

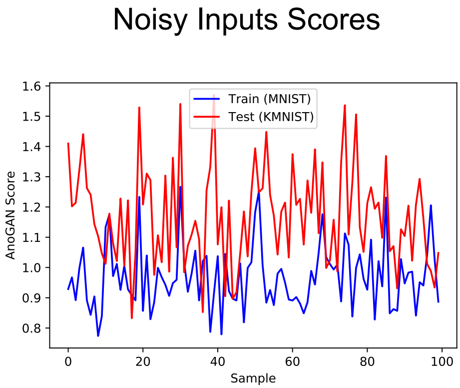
$$\arg\min_{z_\gamma}\{(1-\lambda)\|x - G\left(z_\gamma\right)\| + \lambda BCELoss\left(D\left(G\left(z_\gamma\right)\right), 1\right)\}$$

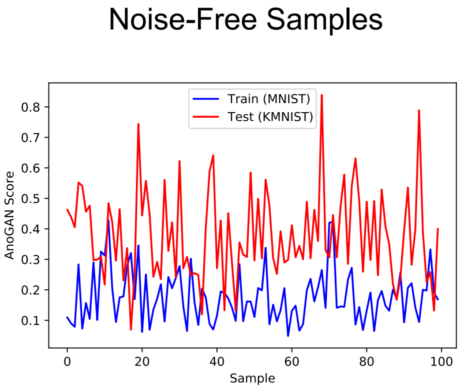
See https://github.com/sulcantonin/ICFA-Beam-2022/blob/main/gan.ipynb

GAN and AnoGAN Example



GAN and AnoGAN Example





Thank you!

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