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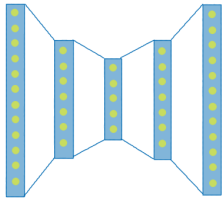
Data Science and Computational Intelligence



UNIVERSIDAD DE GRANADA

# Autoencoders: An Overview and Applications

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SOMACHINE

IAA INSTITUTO DE ASTROFÍSICA DE ANDALUCÍA · EXCELENCIA SEVERO OCHOA · CSIC

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Motivation

Definition

Example

Applications

Current situation and future

# Representation of data sets

Let us organize our data onto a table:

| | | variables → | | | |
|---|---|---|---|---|---|
| | | $A_1$ | $A_2$ | ... | $A_n$ |
| samples ↓ | sample 1 | $v_{11}$ | $v_{12}$ | | $v_{1n}$ |
| | sample 2 | $v_{21}$ | $v_{22}$ | | $v_{2n}$ |
| | sample 3 | $v_{31}$ | $v_{32}$ | | $v_{3n}$ |
| | ⋮ | | | ⋱ | |
| | sample $k$ | $v_{k1}$ | $v_{k2}$ | | $v_{kn}$ |

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- Dimension is the number of variables ($n$). Can it pose a problem?
- Are variables related?

# Curse of dimensionality

What problems can arise as dimension increases?

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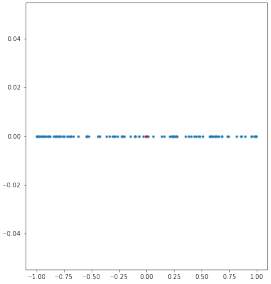
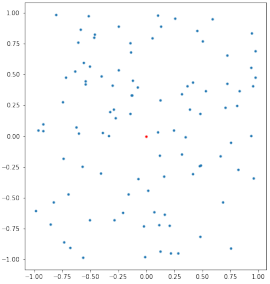
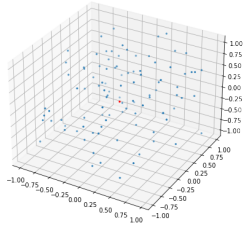



1D




2D




3D

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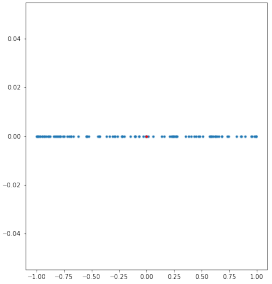
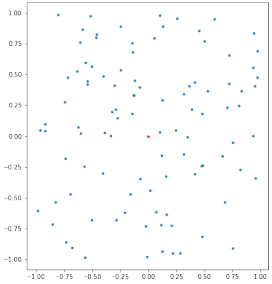
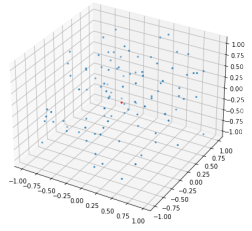



1D




2D




3D

Less fraction of the space is covered by the same amount of data

# Curse of dimensionality

How do distances behave when dimension is high?

[1] C. C. Aggarwal, A. Hinneburg, and D. A. Keim, “On the surprising behavior of distance metrics in high dimensional space,” in *International conference on database theory*, pp. 420–434, Springer, 2001

# Curse of dimensionality

How do distances behave when dimension is high?

$\mathcal{F}$ being a probability distribution of $k$ points. We define the following values:

- $\text{Dmax}_n^p = \max\{\|x\|_p : x \text{ is a sample of } \mathcal{F}^n\}$
- $\text{Dmin}_n^p = \min\{\|x\|_p : x \text{ is a sample of } \mathcal{F}^n\}$

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**Theorem** [1]

There exists a positive constant $C_p$ depending solely on $p$ and verifying:

$$C_p \leq \lim_{n \to +\infty} \mathrm{E}\left[\frac{\text{Dmax}_n^p - \text{Dmin}_n^p}{n^{\frac{1}{p}-\frac{1}{2}}}\right] \leq (k-1)C_p$$

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# Consequences

As $n \to \infty$, the difference between the maximum and the minimum distances to the reference point:

- tends to $\infty$ in the case of the Manhattan distance ($p = 1$)
- tends to a constant for the Euclidean distance ($p = 2$)
- tends to 0 for any p-distance $p > 2$

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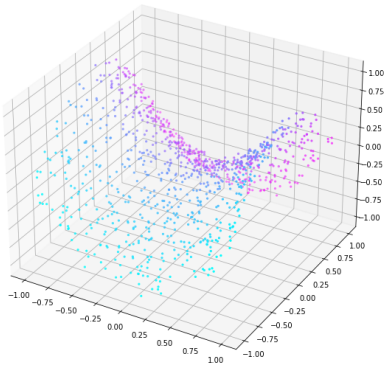
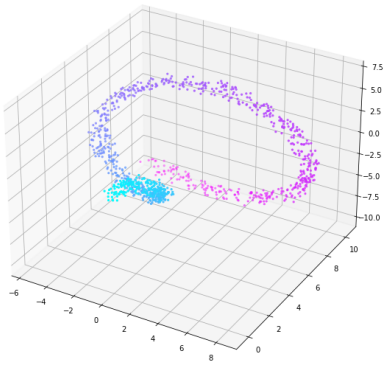
**Most distance metrics lose significance as dimension increases**

# Data in a manifold



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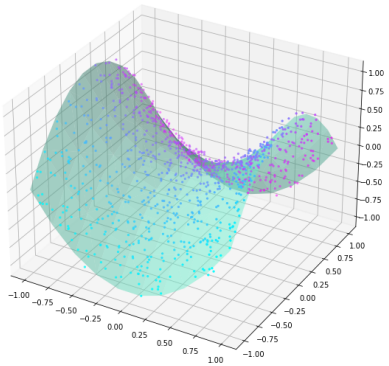


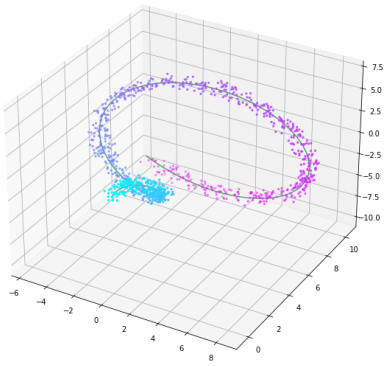


Data is usually not distributed uniformly, but may be found on a manifold

# Alternative representations for problem solving

A better encoding of data samples can simplify:

- Supervised classification
- Unsupervised classification/Semantic hashing
- Anomaly detection
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**Learning a representation of instances can serve as a tool to solve other problems**

This task can be called feature learning, feature extraction, representation learning...

# Unsupervised problem

Supervised tasks involve knowing the solution of a (training) set of instances.

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In our case, the solution is generally **unknown** even for training data.

The best codifications are not known during learning

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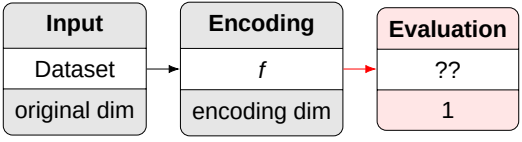
# Input and output

Our encoding learning problem consists in finding a mapping $f : X \rightarrow Z$

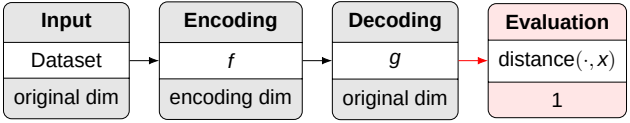
- The **input** is each sample $x \in X$
- The **output** is the encoding $z \in Z$

What is the objective function?



# Supervising the output

Since the only information we have is the input data, use it to provide a fitness score for the encoding: find another mapping $g : Z \to X$ so that $\|g(f(x)) - x\|$ is minimized.



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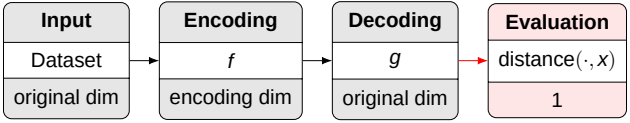


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- Common information (manifold structure) is held by the network weights

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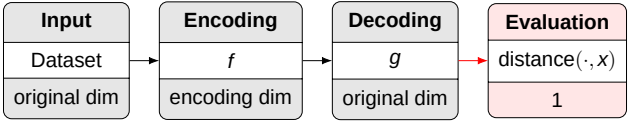


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An **encoder-decoder architecture** can use the inputs as an evaluation tool

# Defining *f* and *g*

Are *f* and *g* any function? No, but they **may approximate any in** $C(I^n)$.

**Theorem (universal approximation)**[2]

There is a single hidden layer feedforward network that approximates any measurable function to any desired degree of accuracy on some compact set *K*.

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This result can be extended to:

- multi-layer networks
- other activation functions

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# Defining $f$ and $g$

$$f = f_k \circ \cdots \circ f_1, \text{ where } f_i(x) = \sigma_i\left(W_i x + b_i\right)$$

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(This is good for parallel computation!)

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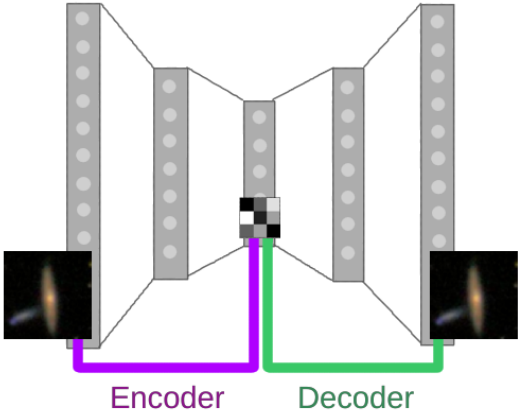
**The encoder and decoder are compositions of matrix products and nonlinearities**

(This is good for parallel computation!)

(What about convolutions? They can be expressed as matrix products)

# Autoencoder architecture



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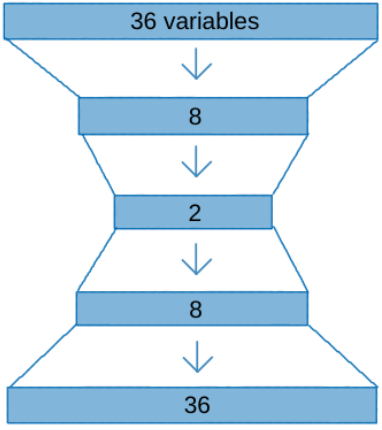
# Example: satellite imagery

Objective: group pixels of an image according to the **type of land** they contain.
For each pixel we have multi-spectral values for the neighboring 8 pixels and itself: in total, 9 pixels $\times$ 4 bands $=$ **36 features**.

| | Aattr | Battr | Cattr | Dattr | Eattr | Fattr | A1attr | B2attr | C3attr | D4attr | E5attr |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.117596 | 1.241362 | 1.184036 | 0.815302 | -0.158561 | 1.256483 | 1.193546 | 0.818486 | -0.141965 | 0.879481 | 0.670010 |
| 2 | -1.205362 | -1.249654 | -0.077532 | 0.444886 | -0.895959 | -0.447579 | -0.786760 | -0.554203 | -0.364672 | 0.092157 | -0.051291 |
| 3 | 0.779075 | 0.148811 | 0.042617 | -0.243030 | 0.800057 | 0.164136 | 0.053370 | -0.448612 | 0.154978 | -0.345245 | -0.712483 |
| 4 | 1.146564 | 0.585831 | 0.342991 | 0.021553 | 0.947536 | 0.601074 | 0.353416 | 0.026550 | 1.788164 | 1.010702 | 0.910444 |
| 5 | -0.764376 | -1.162250 | -0.137607 | 0.180303 | -0.969698 | -1.146681 | -0.126658 | 0.184937 | -0.735851 | -1.132569 | -0.111399 |
| 6 | -0.470385 | -0.725230 | -1.158877 | -1.036778 | -0.232300 | -0.534967 | -1.386853 | -1.029365 | -0.216201 | -0.170284 | -1.133242 |
| 7 | -1.425855 | -1.337058 | -1.279026 | -0.719279 | -1.190918 | -1.321457 | -1.506872 | -0.712591 | -1.403973 | -1.307530 | -1.253459 |
| 8 | -0.911371 | -1.249654 | -1.939848 | -1.513027 | -1.190918 | -1.496232 | -2.106965 | -1.715710 | -0.884323 | -1.220050 | -1.914651 |
| 9 | -1.719846 | -2.036290 | 1.184036 | 2.349882 | -1.707096 | -2.239028 | 1.193546 | 2.560745 | -1.700916 | -2.138594 | 1.210986 |
| 10 | -0.764376 | -0.856336 | 0.042617 | 0.497802 | -0.748479 | -1.102987 | 0.293407 | 0.924077 | -0.735851 | -1.088829 | 0.309360 |
| 11 | 0.779075 | 0.323619 | -0.498055 | -0.825112 | 0.505098 | 0.164136 | -0.486714 | -0.659795 | 0.154978 | 0.004676 | -0.712483 |
| 12 | 1.146564 | 0.585831 | 0.102692 | -0.137197 | 1.168756 | 0.601074 | 0.653462 | -0.131838 | 0.971571 | 0.835741 | 0.670010 |
| 13 | 0.999568 | 0.848043 | 0.342991 | 0.180303 | 1.021276 | 0.863238 | 0.653462 | 0.026550 | 1.045807 | 0.704520 | 0.129035 |
| 14 | -0.176394 | 1.197660 | 0.883663 | 0.603635 | -0.158561 | 0.994319 | 1.193546 | 0.765690 | -0.141965 | 1.010702 | 0.910444 |
| 15 | 1.367057 | 0.804341 | 0.403065 | 0.233219 | 1.684934 | 1.387565 | 0.713472 | 0.448916 | 1.713929 | 1.404364 | 0.970552 |
| 16 | -0.249892 | 1.285064 | 1.063887 | 0.921135 | 0.062659 | 1.300177 | 1.373574 | 1.082464 | 0.080742 | 1.316883 | 1.391311 |
| 17 | -0.249892 | 1.285064 | 1.063887 | 0.709468 | 0.062659 | 1.125401 | 1.373574 | 0.924077 | -0.216201 | 1.141922 | 1.391311 |
| 18 | -0.470385 | 0.848043 | 0.643364 | 0.391969 | -0.748479 | 0.688462 | 0.653462 | 0.396120 | -0.735851 | 0.529559 | 0.670010 |

Let us study a simple solution using **Keras** and an autoencoder.

# Example: satellite imagery




Input

Dense

Dense

Dense

Dense

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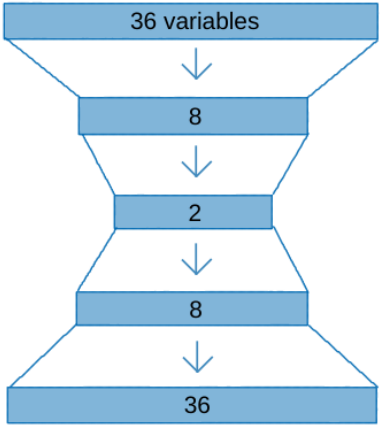


```
Input(shape=(36,))

Dense(8                    )

Dense(2                    )

Dense(8                    )

Dense(36                       )
```

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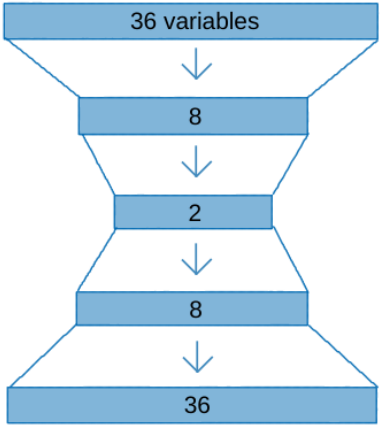



```
Input(shape=(36,))

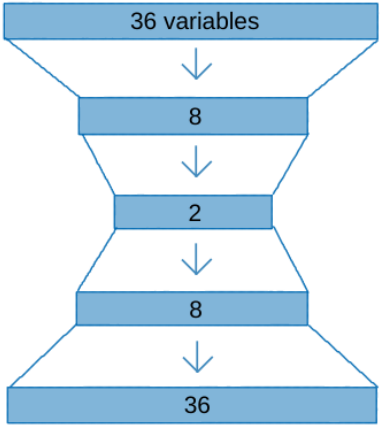
Dense(8, activation='selu')

Dense(2, activation='selu')

Dense(8, activation='selu')

Dense(36, activation='linear')
```

# Example: satellite imagery




```
il = Input(shape=(36,))

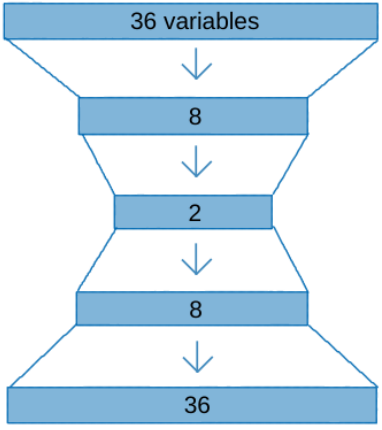
encoder = Sequential([
Dense(8, activation='selu'),


Dense(2, activation='selu')])

decoder = Sequential([
Dense(8, activation='selu'),


Dense(36, activation='linear')])
```

# Example: satellite imagery

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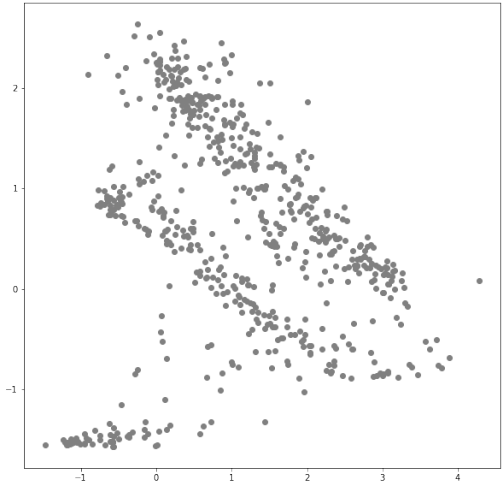
autoencoder =
  Sequential([encoder, decoder])
```

# Test encodings

After training and selecting a model, we can obtain codes for other samples.

Codes can be used for visualization and clustering.

The (SGD-based) optimizer can produce different results in different runs.

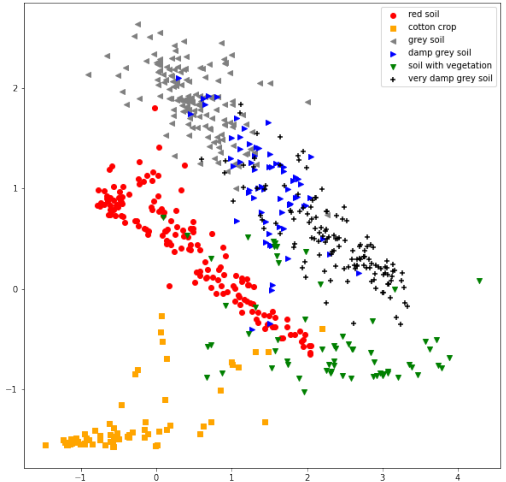


# Test encodings

After training and selecting a model, we can obtain codes for other samples.

Codes can be used for visualization and clustering.

The (SGD-based) optimizer can produce different results in different runs.



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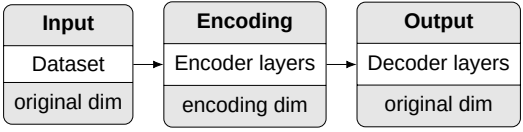
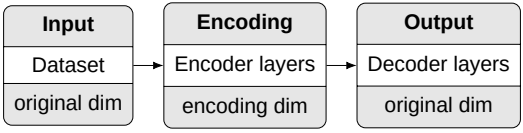
# Reminder: general structure



# Reminder: general structure

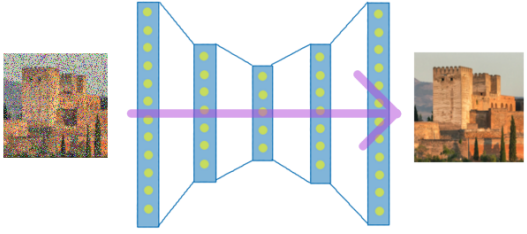



We need 3 Keras models:

- `encoder`: layers up to encoding → encode data
  `Model(data_input, encoding)`
- `decoder`: layers from encoding → generate new data
  `Model(code_input, reconstruction)`
- `autoencoder`: composition of models → train/reconstruct
  `Sequential([encoder, decoder])`

# Noise reduction: strategy

- **Objective**
  Improve manifold modeling and reduce noise
- **Method**
  Input noisy data and evaluate over clean data
- **Reference**
  Vincent et al. *Extracting and composing robust features with denoising autoencoders*. In Proceedings of the 25th international conference on Machine learning (pp. 1096-1103).



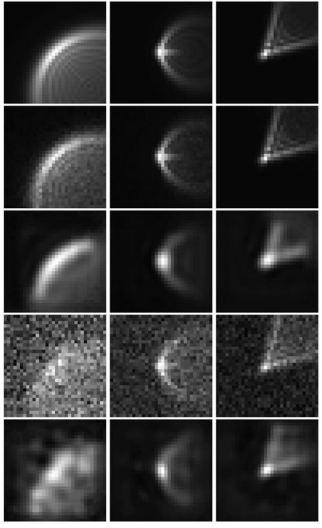
# Convolutional denoising autoencoders for noise reduction

Case study: **denoising a 10-class object classification dataset**

| Noisy input | | Encoding | | Output |
|---|---|---|---|---|
| STL10 + noise | Conv $(5 \times 5)$ | Max pooling $(2 \times 2)$ | Deconv $(5 \times 5)$ | Upsampling $(2 \times 2)$ | Deconv $(3 \times 3)$ |
| $96 \times 96 \times 3$ | $96 \times 96 \times 64$ | $96 \times 96 \times 128$ | $48 \times 48 \times 128$ | $48 \times 48 \times 64$ | $96 \times 96 \times 64$ | $96 \times 96 \times 3$ |

# Convolutional denoising autoencoders for noise reduction

Figure 6.



From the literature: **point spread function modelling**

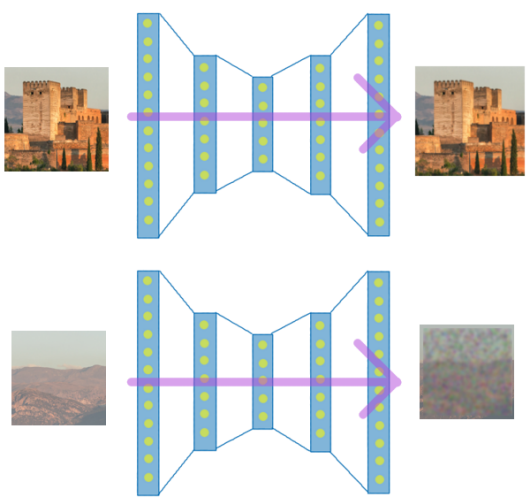
Jia, P., Li, X., Li, Z., Wang, W., & Cai, D. (2020). Point spread function modelling for wide-field small-aperture telescopes with a denoising autoencoder. Monthly Notices of the Royal Astronomical Society, 493(1), 651-660.

# Anomaly detection: strategy

- **Conjecture**
  An autoencoder trained on *normal* data cannot reconstruct anomalous data

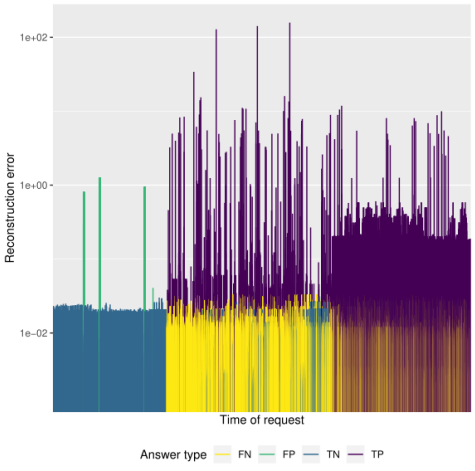
- **Method**
  Anomaly score = reconstruction error

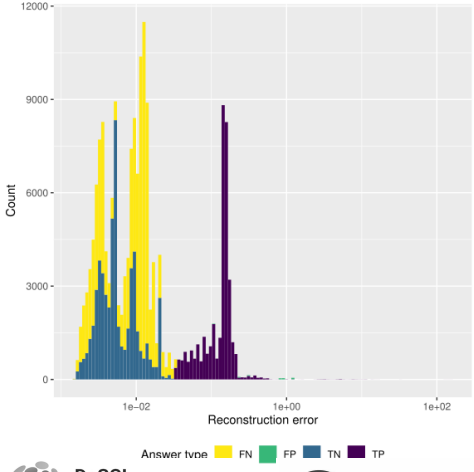
- **Reference**
  Sakurada et al. *Anomaly detection using autoencoders with nonlinear dimensionality reduction*. In Proceedings of the MLSDA 2014 2nd Workshop on Machine Learning for Sensory Data Analysis (pp. 4-11).



# Denoising autoencoders for anomaly detection

Case study: **attack detection in networks**

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# Denoising autoencoders for anomaly detection

## From the literature: **gravitational wave detection**

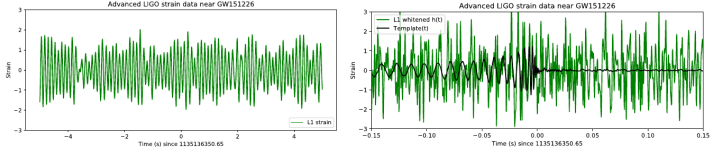



**Fig. 1.** (left) Example of a time series containing a GWs signal immersed in LIGO noise (ID GW151226). Since data are dominated by noise, it is not possible to see the signal without some signal processing. (right) Whitened time series containing a GWs signal (ID GW151226) and the best matching template identified in the LIGO search pipeline.

Corizzo, R., Ceci, M., Zdravevski, E., & Japkowicz, N. (2020). Scalable auto-encoders for gravitational waves detection from time series data. Expert Systems with Applications, 113378.

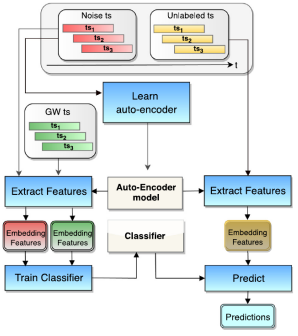



**Fig. 5.** Workflow of the AE-FE proposed method. Negative class time series (red) are exploited to train an auto-encoder model that accurately reconstructs noisy time series. The auto-encoder encodes both negative class (red) and positive class (green) time series and the resulting representation is used to train a classifier. At prediction time, a new time series of unknown class (yellow) is provided to the classification model, which returns its prediction.

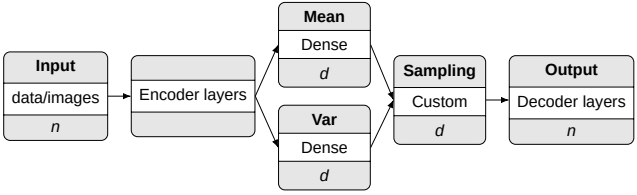
# Instance generation: strategy

- **Objective**
  Use a trained decoder to generate plausible unseen data
- **Method**
  Learn probability distributions instead of codes
- **Reference**
  Kingma, Diederik P., and Max Welling. “Auto-encoding variational bayes.” arXiv preprint arXiv:1312.6114 (2013).

ThisPersonDoesNotExist.com

# Generative autoencoders for instance generation

Basic variational autoencoder structure:




*Reparametrization trick*: estimate a sample from $\mathcal{N}(\mu, \Sigma)$ using one from $\mathcal{N}(0, I)$.

With 1 variable: $z' = \mu + \sigma z$

# Generative autoencoders for instance generation

From the literature: **galaxy deblending**

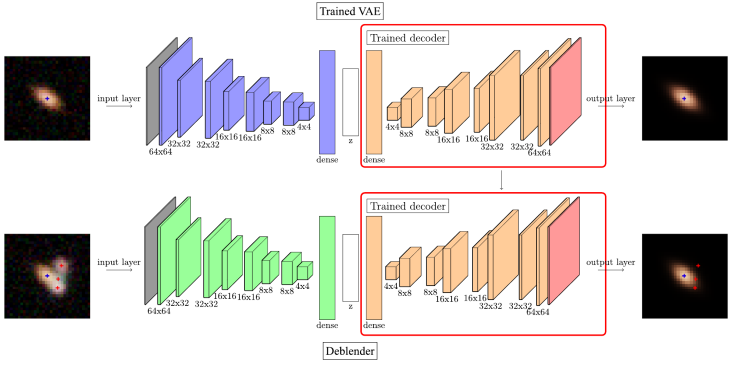



**Figure 3.** Architectures of the VAE and the deblender. The weights of the VAE's trained decoder are loaded and fixed in the deblender network before training.

B. Arcelin et al., "Deblending galaxies with variational autoencoders: A joint multiband, multi-instrument approach," Monthly Notices of the Royal Astronomical Society, vol. 500, no. 1, pp. 531–547, 2020

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# Software packages

Deep learning libraries:

- Tensorflow/Keras
- PyTorch

Generic implementations of autoencoders are scarce:

- Ruta (for R) https://ruta.software
- autoencoder (Python)

Many specific implementations for concrete applications

# What's next?

- Many variants of generative autoencoders (VAE, Adv. AE)
- **Transformers**
  A. Vaswani et al., "Attention is all you need," in Advances in neural information processing systems, pp. 5998–6008, 2017

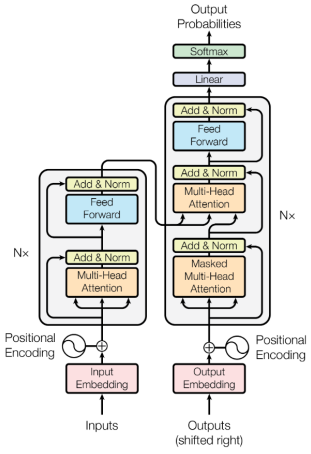


Figure 1: The Transformer - model architecture.

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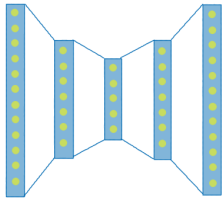

UNIVERSIDAD DE GRANADA

# Autoencoders: An Overview and Applications

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SOMACHINE

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