Karlsruhe Institute of Technology

Data Driven Engineering I: Machine Learning for Dynamical Systems

Introduction to Generative Learning: Autoencoders

Institute of Thermal Turbomachinery
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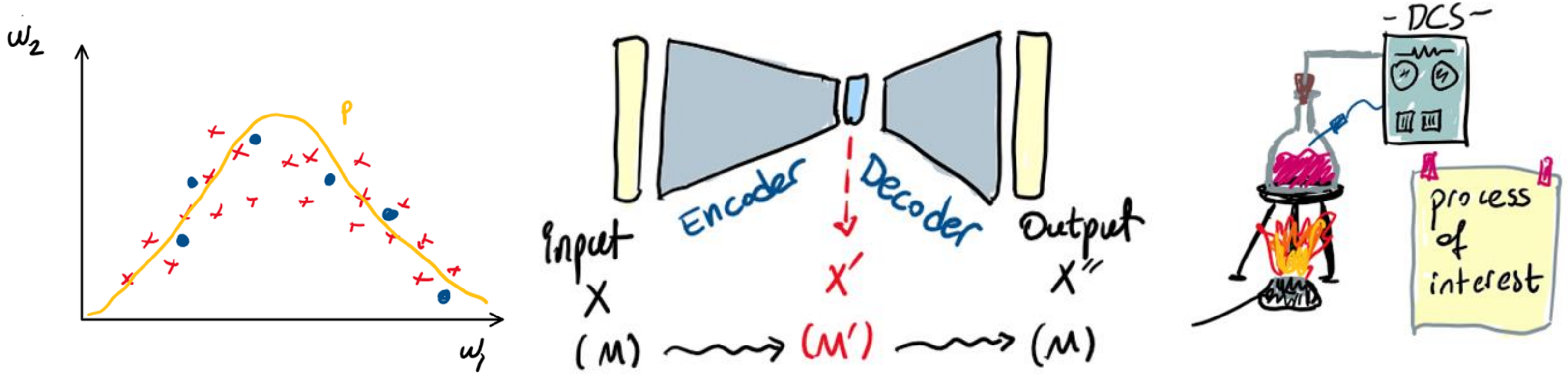


Previously on DDE-1 :

* Supervised learning → Classification
  → Regression

* Unsupervised learning → Clustering
  → Dim. Reduction

+ Deep Learning

+ Time Series Analysis

Models we have discussed so far...

* Supervised learning

⇒ $\left.\begin{matrix}[X] \\ y\end{matrix}\right\}$ Learn a function to map $[X] \rightarrow y$ } "Discriminative models"

* Unsupervised learning

⇒ $[X] \rightleftarrows [X]$ learn some underlying hidden structures

⇒ Feature Extraction ?

⇒ Promising ⇐ $[X]$ "available"

UL → Generative Models :

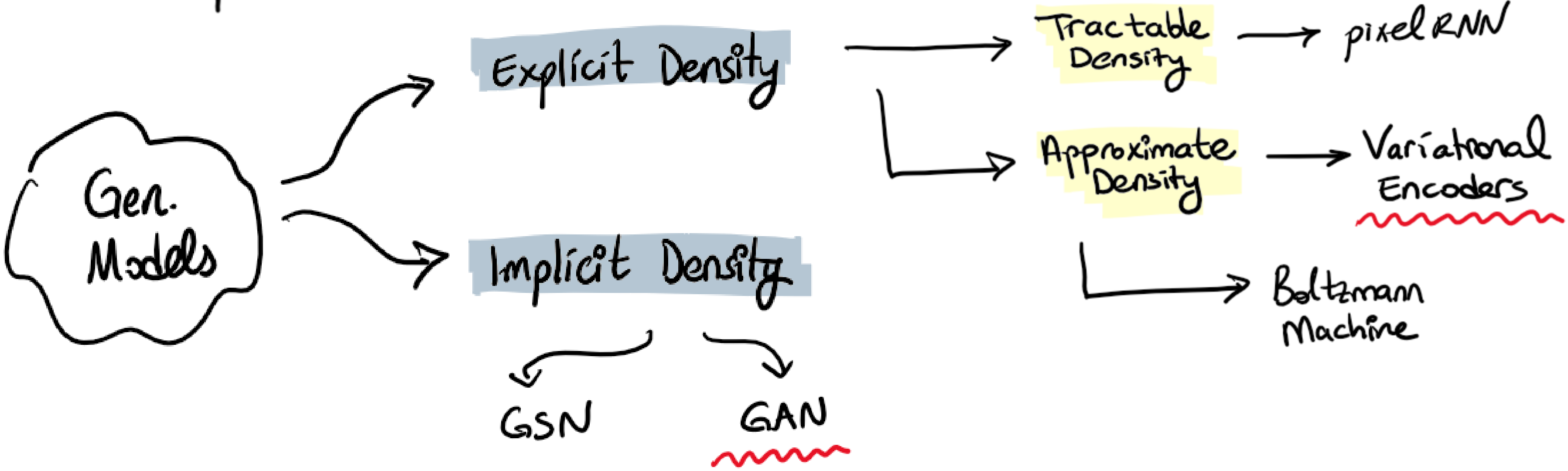
- model tells how [x] is formed at the beginning
- It is probabilistic in nature
    - StyleGAN
    - GPT language model
    - Virtual training → (RL)

UL → Generative Models :



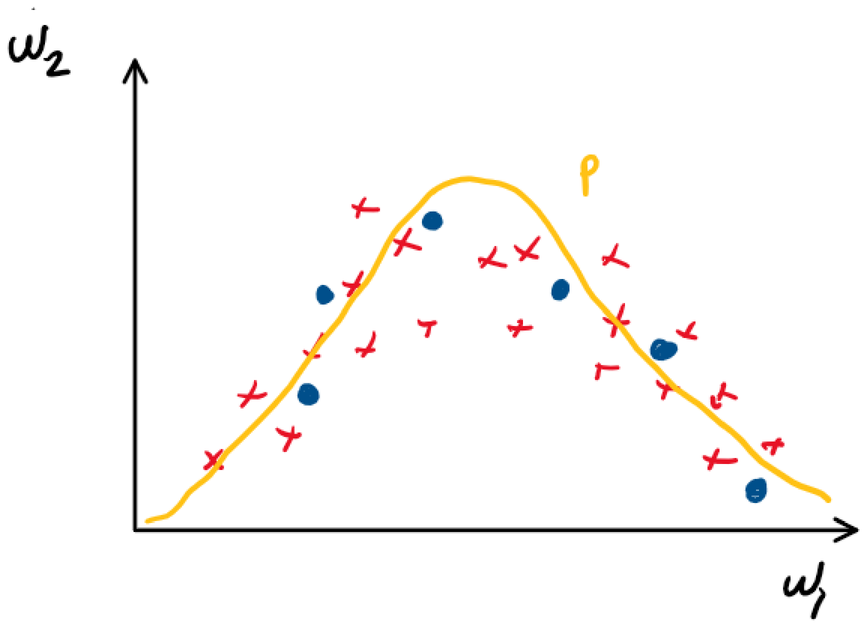

UL → Generative Models :

* It is probabilistic in nature



How does it work?

- ☑ we have a dataset X.
- ☑ we assume that it is generated according to a rule p
- ☑ Model mimics p to create new points.
- ☑ Model should not reproduce what it has seen.



How does it work?

① **Sample space**: Values an observation can take $x = [\cdots]$

② **Probability Density Function**: function maps x in sample space; $PDF = [0, 1]$

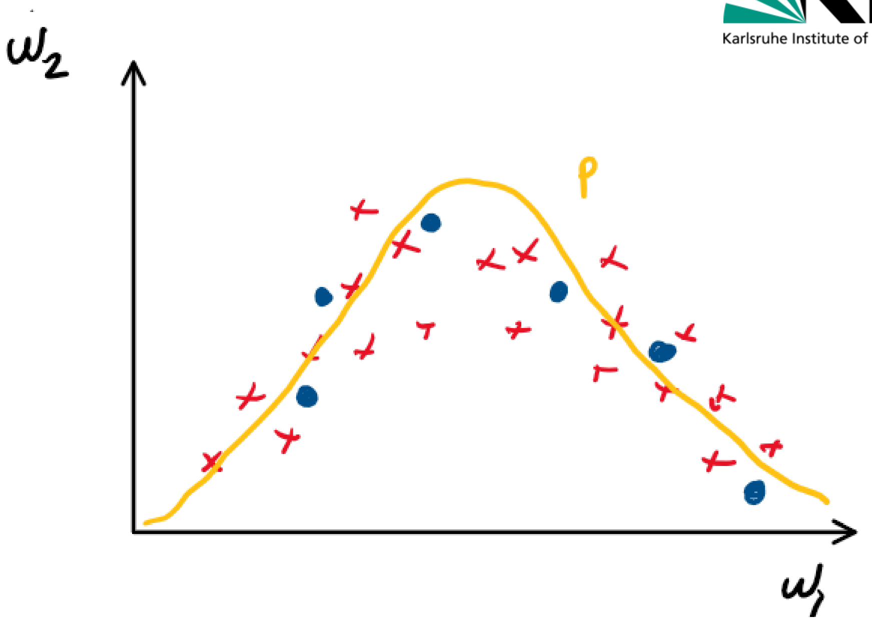
it is well-defined $\Rightarrow$ $\int PDF = 1.0$

③ **Parametric Modeling**: $p_\theta(\underbrace{\theta_1, \theta_2, \theta_3}_{\text{find } [\theta_i]}) \longrightarrow$ true p

$\Rightarrow$ "maximum likelihood estimation"

How does it work?

- [x] we have a dataset X.
- [x] we assume that it is generated according to a rule p
- [x] Model mimics p to create new points.
- [x] Model should not reproduce what it has seen.



- [ ] how can we infer the rules (p_θ) from data?

↳ Representation Learning

Representation Learning

[X] $\Longrightarrow$ [X']

high dim. (M) space

low dim. space (M')

} latent space

$\Rightarrow$ learn p_θ $\Rightarrow$ learn p'_θ

Eg.

2 47 16 14 21

72 71 70 69 68 67 66 65 64 63 62 61 60 59 58 57

5 # ✓

16 # ✗

(72, 57, 1) → ✗

→ ✓

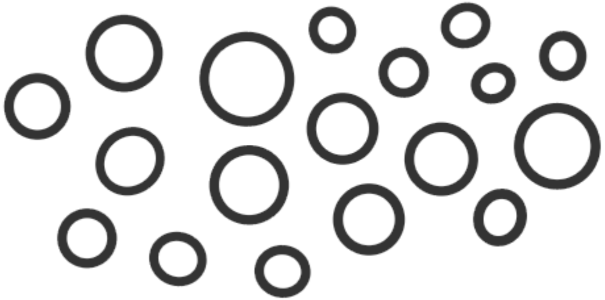
Representation Learning

$[X] \Longrightarrow [X']$ } latent space ⇨ learn p_θ ⇒ learn p'_θ

high dim. (M) space — low dim. space (M')

Perception in chess, 1973

Eg



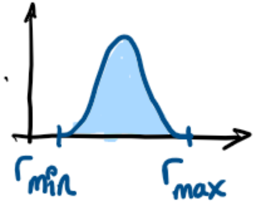
x_0 = 'circle'

$x_1 = (r_0, r_1, r_2, \ldots r_N)$

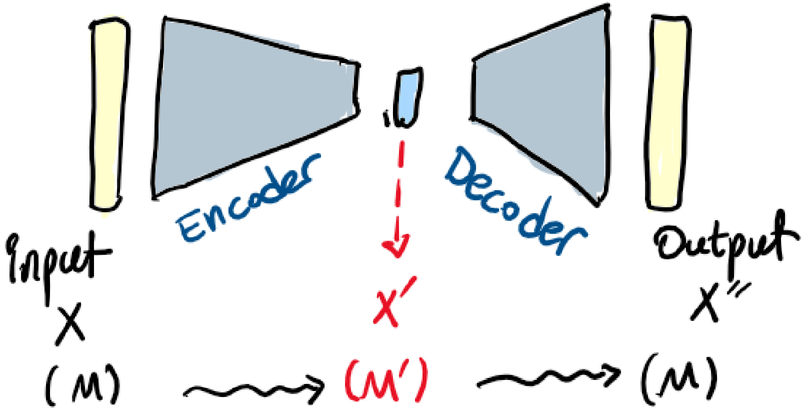
Task: Draw these objects!

Gen. Model

$[X] \rightarrow \boxed{} \rightarrow$ Circle, $p_\theta = \phi_r$

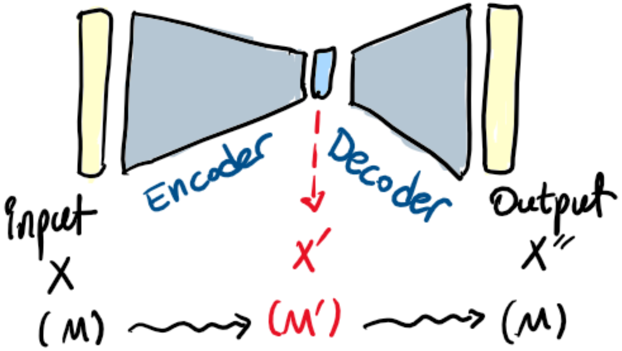


Autoencoders :

- unsupervised approch
- Obj : lower dim. representation (higher ?)
- 

- Reconstructed X''
- By-product $\Rightarrow X'$
- Cost function : $\|X''-X\|^2$

Autoencoders :



* Use cases :

- ☑ Dimensionality Reduction
- ☑ Anomaly detection

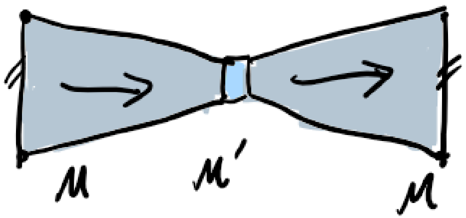
* Use cases :

- ☑ Forecasting ~ generative
- ☑ Sparse Representation
- ☑ Denoising dataset
- ☑ "Interpolator"
- ☑ Unsupervised pre-training
- ☑ "Generative Model" (+ pdf)

Base model: Under-complete linear AE

* MLP → linear activation function
  ↳ cost := MSE

⇓ $\approx$ PCA

* 

$M > M'$
Symmetrical layer(s)

* Many layers ⇒ Deep Autoencoder
* Good for large [X] with high M.
* can be used for outlier detection

Today's Agenda

Basic Steps to Follow:

0.) Understand the business/task.
1.) Understand the data.
2.) Explore & prepare the data.
3.) Shortlist candidate models.
4.) ~~Training the model~~
5.) Evaluate the model predictions
6.) "Serve" the model !

Still valid

#0 Understanding the task

- ❑ **Problem**: Manufacturing error in a production line
- ❑ **Modified sensory input:** 28 variables including sensory input
- ❑ 280,000 instances, where only a **small fraction** (~500) of products are **defective**.
- ❑ **Heuristic**: <0.5% is defective

A similar example for you:

“Bosch Production Line Performance
Reduce manufacturing failures”

#1 Understanding the data

- ❑ Check the data source: understand what the data refers to
- ❑ Objective: understand the characteristics of the data
- ❑ Look at the feature columns:
  - ❑ Any missing values?
  - ❑ Any features with NaN values?
  - ❑ Uniqueness of the dataset? ("cardinality")

=> Colab

```
 23   S23      284807 non-null  float64
 24   S24      284807 non-null  float64
 25   S25      284807 non-null  float64
 26   S26      284807 non-null  float64
 27   S27      284807 non-null  float64
 28   S28      284807 non-null  float64
 29   Class    284807 non-null  object
dtypes: float64(29), object(1)
memory usage: 65.2+ MB
time: 54.5 ms
```

	Time	S1	S2	S3	S4	S5	S6
count	284807.000000	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05
mean	94813.859575	1.758743e-12	-8.252298e-13	-9.636929e-13	8.316157e-13	1.591952e-13	4.247354e-13
std	47488.145955	1.958696e+00	1.651309e+00	1.516255e+00	1.415869e+00	1.380247e+00	1.332271e+00
min	0.000000	-5.640751e+01	-7.271573e+01	-4.832559e+01	-5.683171e+00	-1.137433e+02	-2.616051e+01
25%	54201.500000	-9.203734e-01	-5.985499e-01	-8.903648e-01	-8.486401e-01	-6.915971e-01	-7.682956e-01
50%	84692.000000	1.810880e-02	6.548556e-02	1.798463e-01	-1.984653e-02	-5.433583e-02	-2.741871e-01
75%	139320.500000	1.315642e+00	8.037239e-01	1.027196e+00	7.433413e-01	6.119264e-01	3.985649e-01
max	172792.000000	2.454930e+00	2.205773e+01	9.382558e+00	1.687534e+01	3.480167e+01	7.330163e+01

time: 447 ms

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#2 Exploring the data

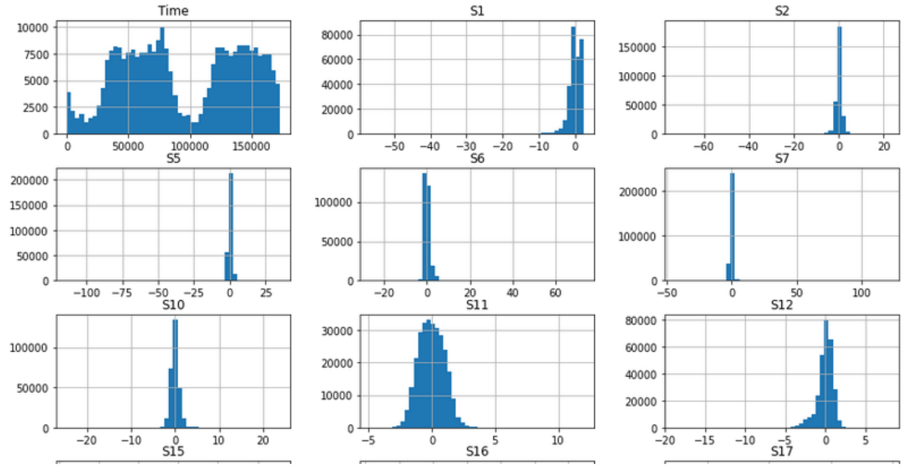
- **Objective**: generate a data quality report

- Using standard statistical measures of central tendency and variation
  - tabular data and visual plots
  - mean, mode, and median
  - standard deviation and percentiles
  - bars, histograms, box and violin plots

✓ Missing values,

✓ Irregular cardinality problems,
  - 1 or comparably small

✓ Outliers
  - invalid outliers and valid outliers



#2 Exporing the data: Correlation Matrix

- Shows the correlation between each pair of features

$$\mathrm{Cov}(a,b) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(a_i-\bar{a})\times(b_i-\bar{b})\right]$$

Features   instance   mean   mean

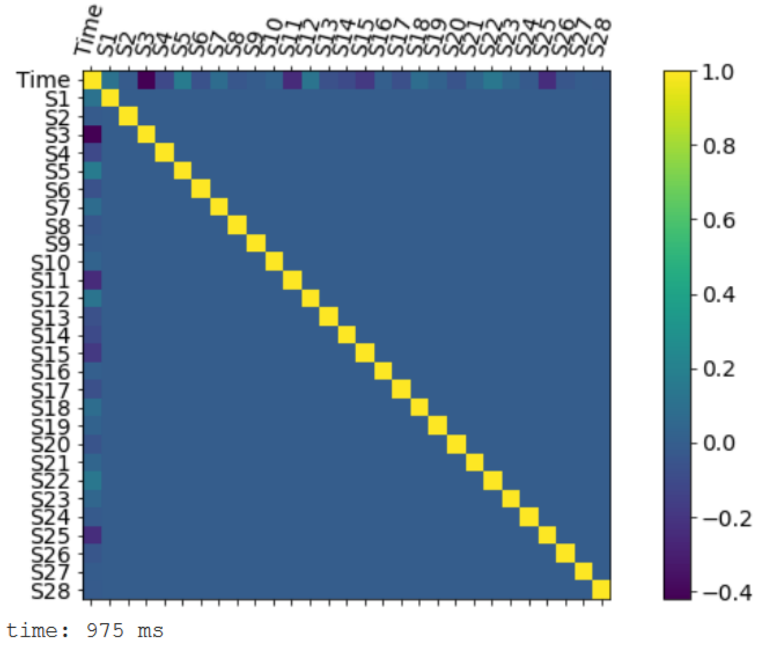
- Normalized form of "covariance"

$$\mathrm{Corr}(a,b) = \frac{\mathrm{Cov}(a,b)}{SD(a)\times SD(b)}$$

* Normalized
* Dimensionless

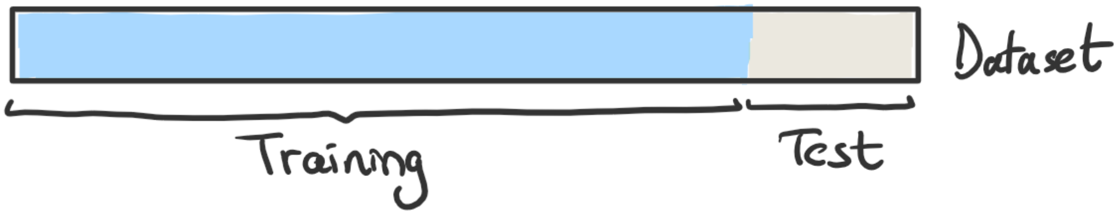
Easy to interpret

- Ranges between −1 and +1



#2 Preparing the Data

- Clustering >> unsupervised >> **training & test split not needed**



- We will use it to **reduce the volume of the data** when needed:

```
[ ]  X_train, X_test, y_train, y_test = train_test_split(dataX,
     dataY, test_size=0.9,
     random_state=2020, stratify=dataY)

     time: 188 ms
```

#5 Evaluating the Results: Reconstruction error

$$X \rightarrow \underbrace{\boxed{D.R.}}_{\text{Encoding}} \rightarrow \tilde{X} \rightarrow \underbrace{\boxed{DR^T}}_{\text{Decoding}} \rightarrow X'$$

X ⇓ physical coordinates

$\tilde{X}$ ⇓ "latent space"

X' ⇓ physical coordinates

if DR is capable of learning the patterns in the physical system;

$$X \approx X'$$

* $$loss = \sum_{m=1}^{M} (x_m - x'_m)^2 \Rightarrow N \text{ elements}$$

Normalization:

* $$loss' = \frac{loss - \min(loss)}{\max(loss) - \min(loss)} \Rightarrow [0, 1]$$

Interpretation:

* $loss' \rightarrow 0$ ⇒ Regular Product

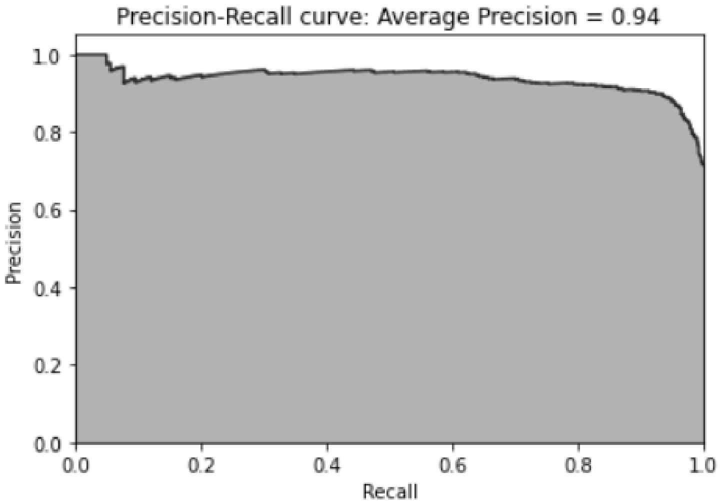
  $loss' \rightarrow 1$ ⇒ Anomaly, defective

#5 Evaluation of the predictions

Precision Recall Curve (for imbalanced data)

$$\text{Precision} := \frac{\text{True Positive}}{\text{TP} + \text{False Positive}} \Rightarrow \frac{\text{It is positive}}{\text{“It is positive”}}$$

$$\text{Recall} := \frac{\text{True Positive}}{\text{TP} + \text{False Negative}} \Rightarrow \frac{\#\,\text{Correct Predict.}}{\#\,\text{True Cases}}$$



- **Precision** captures how often, when a model makes a positive prediction, this prediction turns out to be correct.
- **Recall** tells us how confident we can be that all the instances with the positive target level have been found by the model.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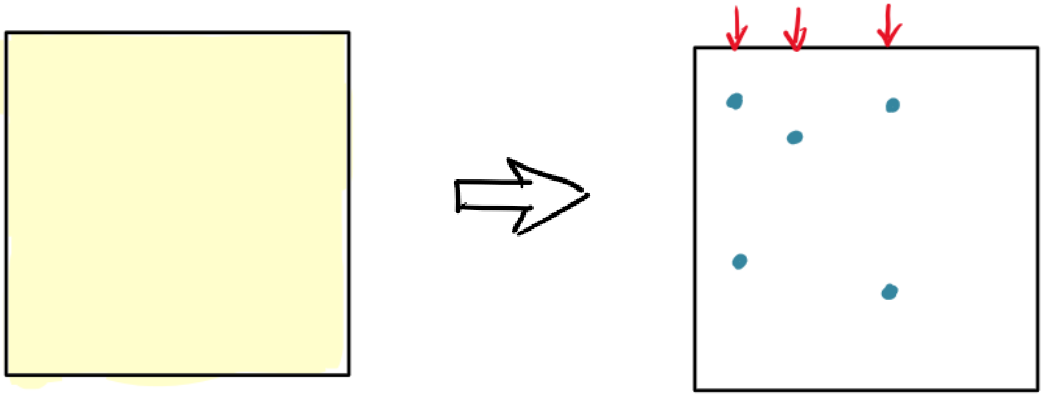
Sparse Autoencoders:

* Sparse matrices

Sparse Representation

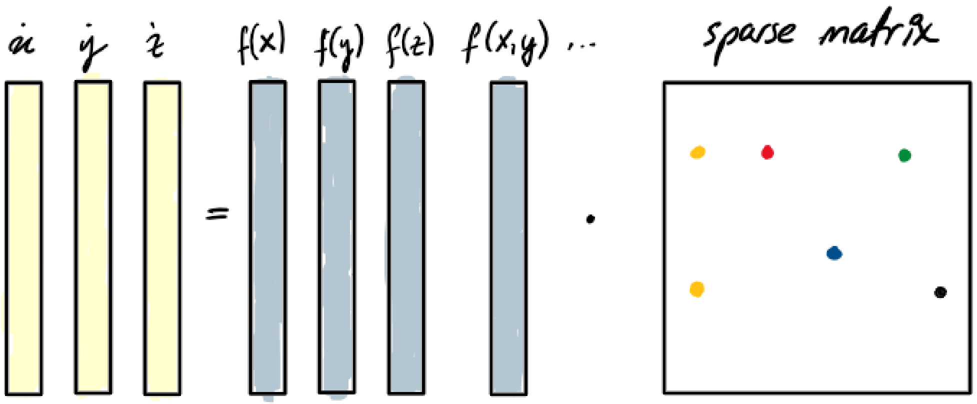
$W =$



every element is important.

⇒ non-zero elements

Data Driven Model Discovery.

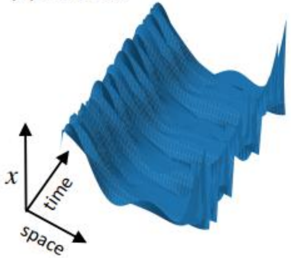


$$\dot{x} = ax - bxy^2 + \phi_i$$
$$\dot{y} = cyz + \phi_i$$
$$\dot{z} = axy + \sin\phi_i$$

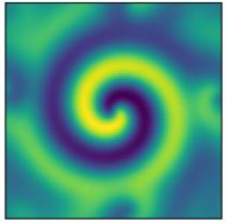
Reg. Linear Regression

$$\dot{z}_1 = -10.0z_1 + 10.0z_2$$
$$\dot{z}_2 = 27.7z_1 - 0.9z_2 - 5.5z_1z_3$$
$$\dot{z}_3 = -2.7z_3 + 5.5z_1z_2$$

(a) Lorenz

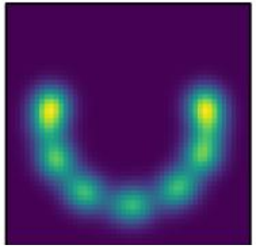


(b) Reaction-diffusion



$$\dot{z}_1 = -0.85z_2$$
$$\dot{z}_2 = 0.97z_1$$

(c) Nonlinear pendulum



$$\ddot{z} = -0.99\sin z$$

Sparse Autoencoders:

* Modify the cost function to enforce sparse "neurons".
  - ↳ l_1 regularization
  - ↳ sigmoid activation functions
  - ↳ large encoders

simpler tools

⇒

(i) have a target sparsity

(ii) measure actual sparsity

(iii) Give penalty

Check average neuron activity in batch.

[KL Divergence]

↳ Add sparsity loss to total loss.

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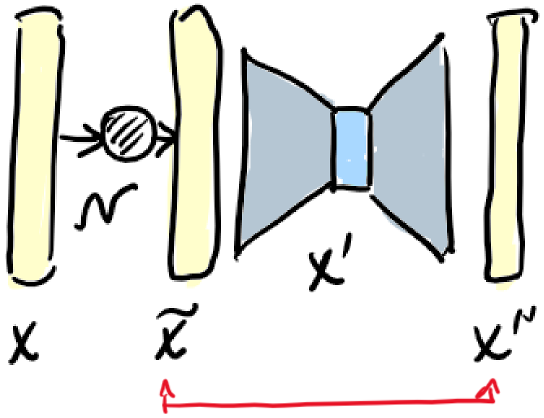
De-noising Your Data:

- PIV Measurements
- Simulation data ⇒ FTLE -



! "Clean data" is needed.

Obj: Learn to clean the data from noise.

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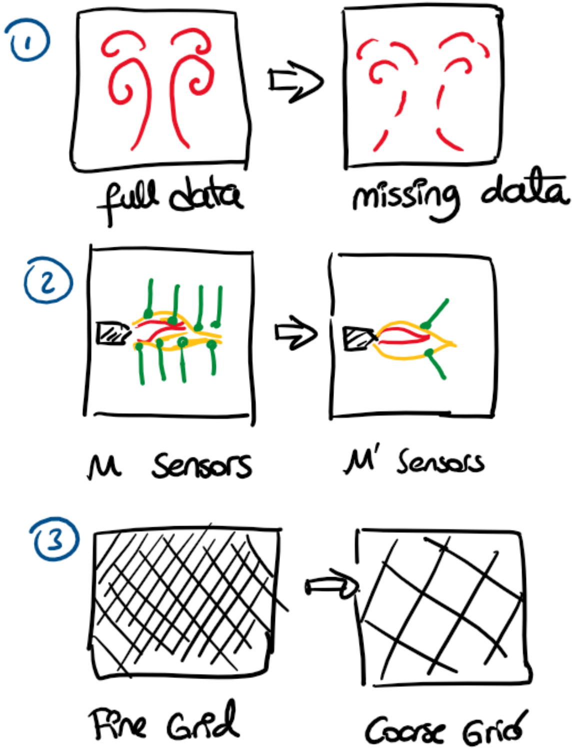
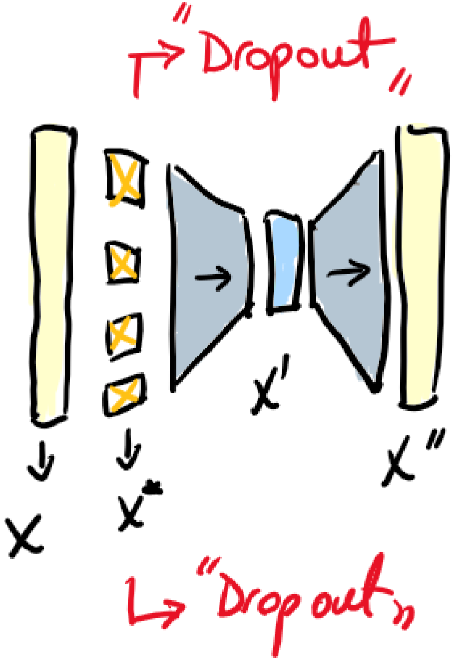
Interpolation Tool:





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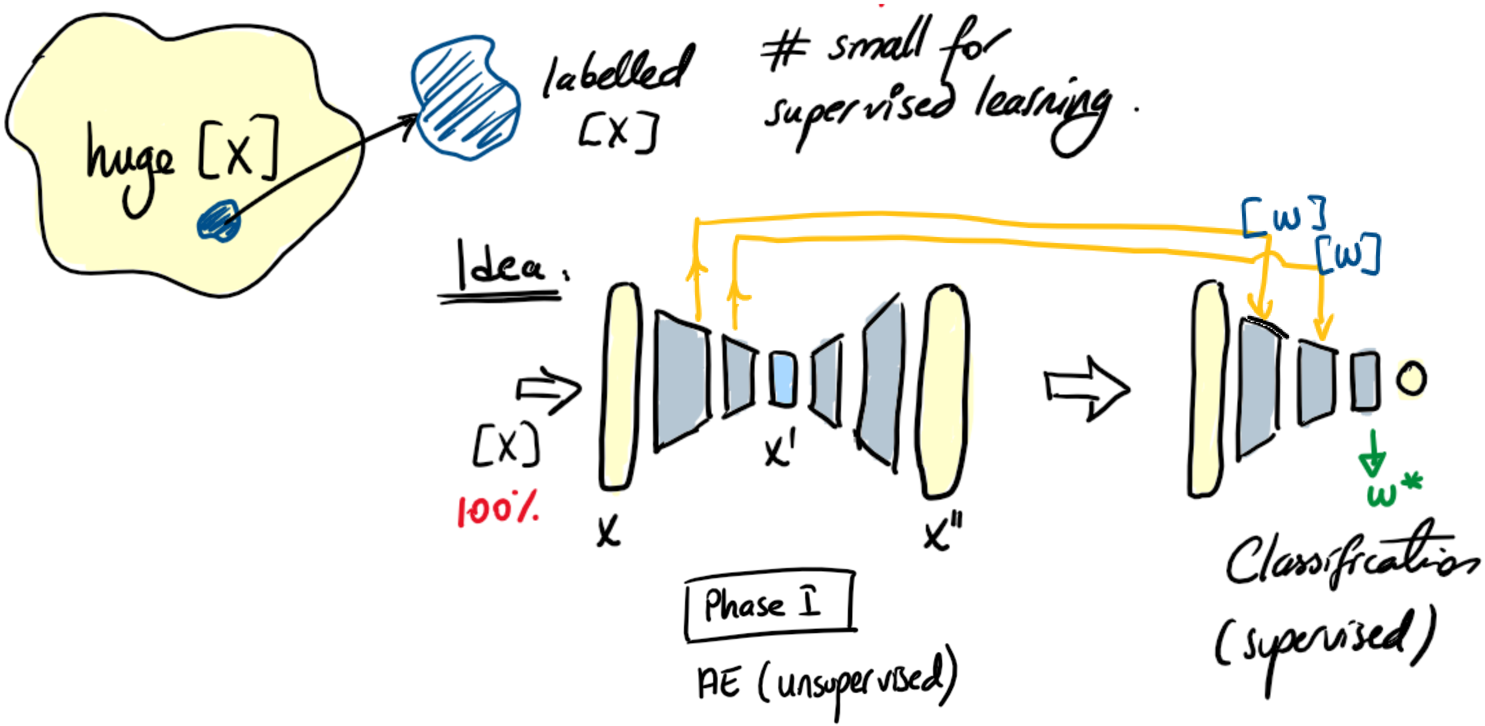
Unsupervised Pretraining



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Additional Notes

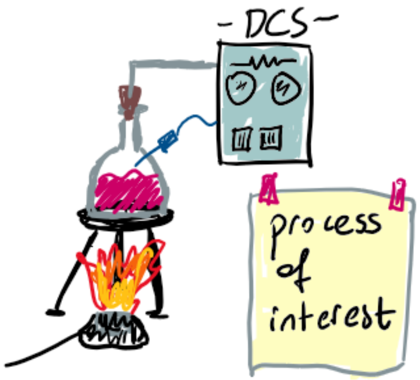
Dim. Reduction:

Computational
– preprocessing –

Feature Extraction
~ pattern recognition ~

Visualization

Idea:



$$X = \begin{bmatrix} — \cdots — \\ — \text{product}_n — \\ — \cdots — \end{bmatrix}$$

→ information in on the production line

Idea:

Assume:

- $product = \sum_{i=1}^{K} process_i$
- Features m is correlated to K steps in the production line;

Then:

$$X \rightarrow \boxed{D.R.} \rightarrow \tilde{X} \rightarrow \boxed{DR^T} \rightarrow X'$$

physical coordinates

"latent space"

physical coordinates

Encoding

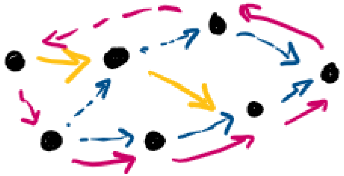
Decoding

if DR is capable of learning the patterns in the physical system;

$$X \approx X'$$

Idea:

Interpreting Patterns



* Physical system is composed of logical steps;
* Logical steps followed ⇒ "Regular product"
* Failure at some point ⇒ "Defect"

"Outlier Detection"

A.I.

"Something is wrong here."

Aim ⇒ Learn enough to detect outliers;