

Artificial Intelligence in Engineering and Sciences

by

Dr Varun Ojha

University of Reading

at

University of Surrey

06 December 2022

Agenda

1. What are the AI Tools?

(scope)

2. What problems do they solve?

(domain)

3. How do they solve problems?

(algorithms)

What we want to know

1. to understand the data

(data collection, processing, and modelling)

2. to make some prediction

(forecasting)

3. to optimize some systems

(discovering appropriate parameters, variables, and settings)

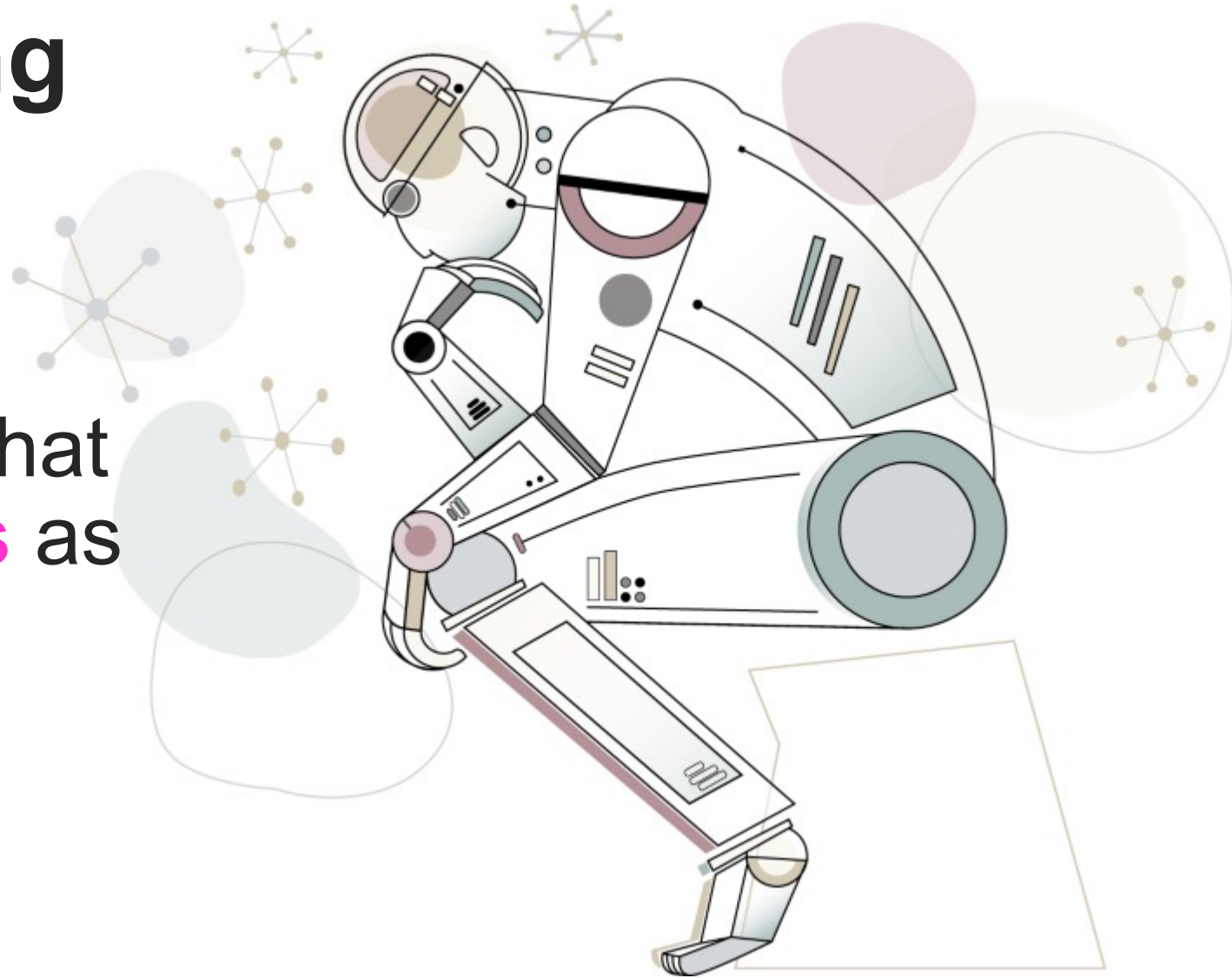
Artificial Intelligence

to create intelligent machines that
think (react) and **act** (work) like
human beings



Machine Learning

to create machines that
learn from examples as
living beings do



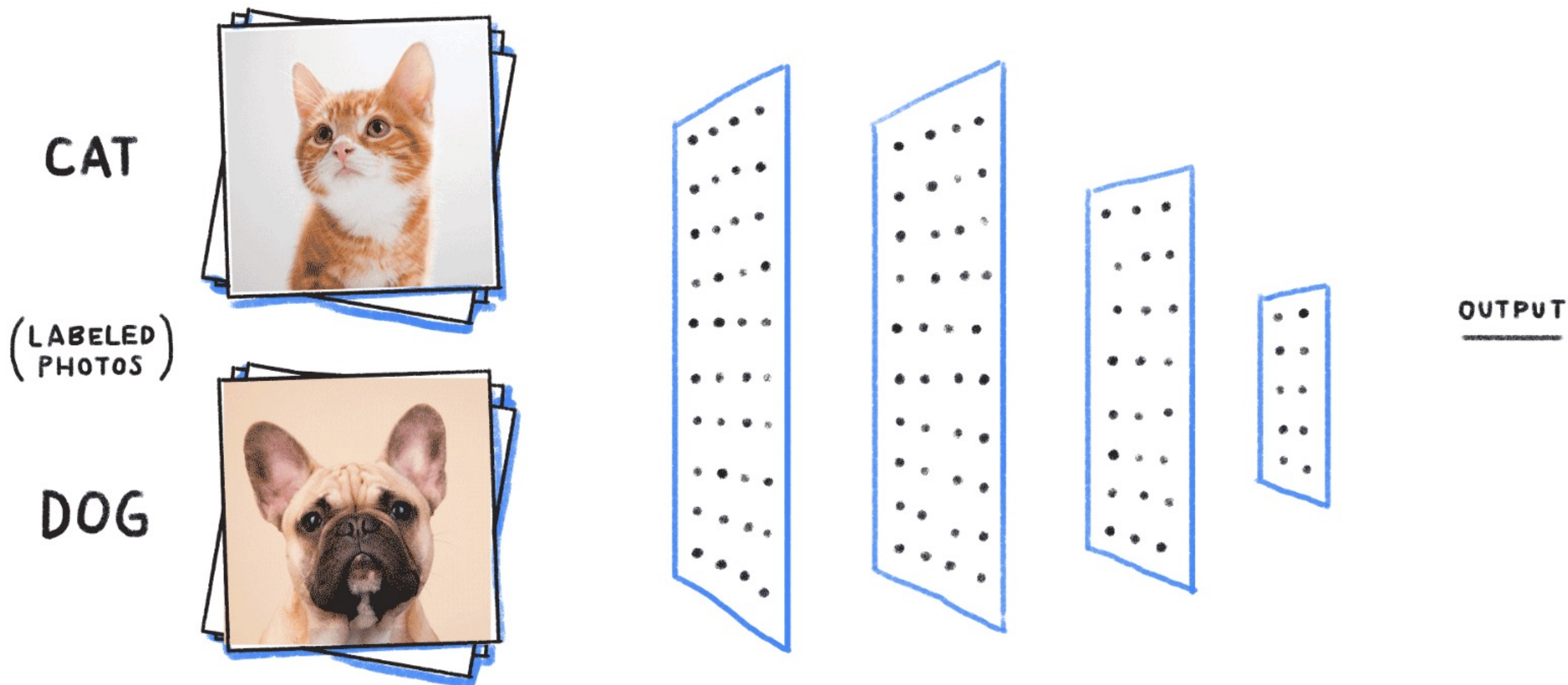
Learning

Video Source:
<https://www.youtube.com/watch?v=Ak7bPuR2rDw>
(Accessed on 21 February 2021)



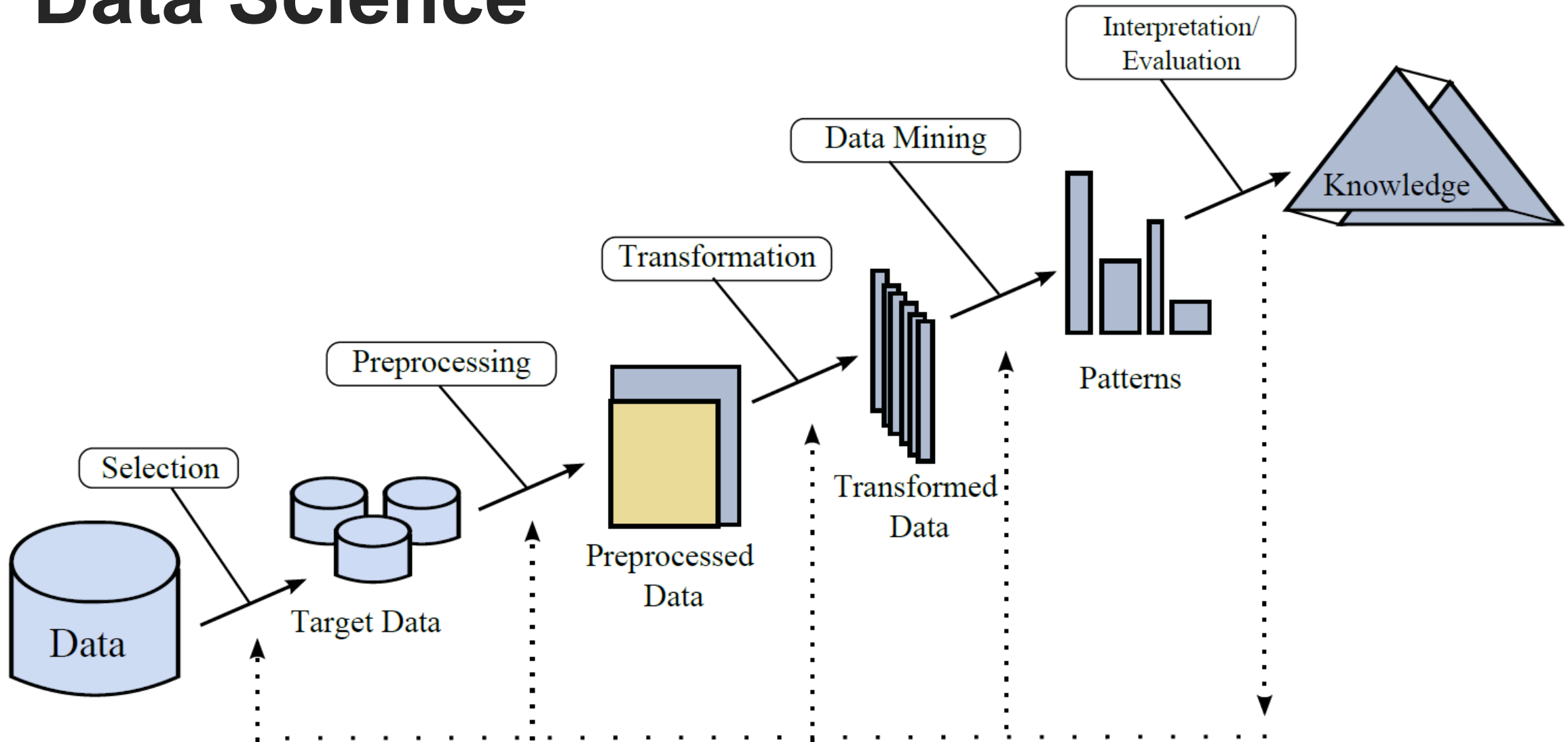
Deep Learning

Source: <https://becominghuman.ai/building-an-image-classifier-using-deep-learning-in-python-totally-from-a-beginners-perspective-be8dbaf22dd8>





Data Science



Optimization



Optimization

to solve a **problem** that has a number of influencing factors that **need to attain certain value** in order to offer a **solution**

Applications of AI

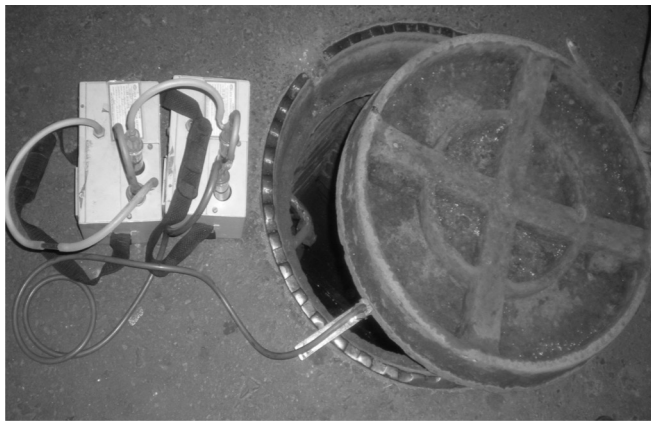
1. Engineering
2. Pharmacy & Drugs
3. Environment (Physiology & Architecture)
4. Civil Engineering
5. Physics
6. Biology
7. Hydrology
8. Climate Science

Electronics Engineering

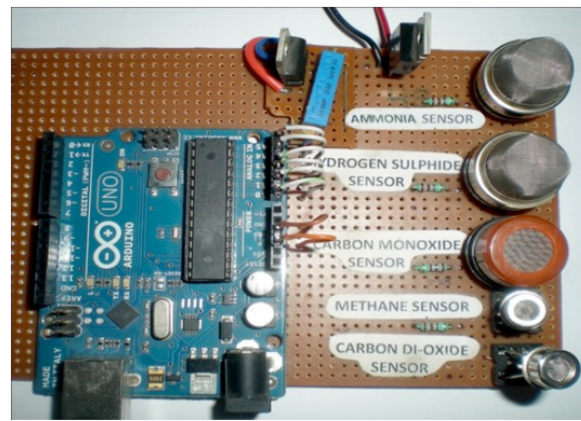
Protection of health and life of sewer pipeline workers

Pattern Recognition

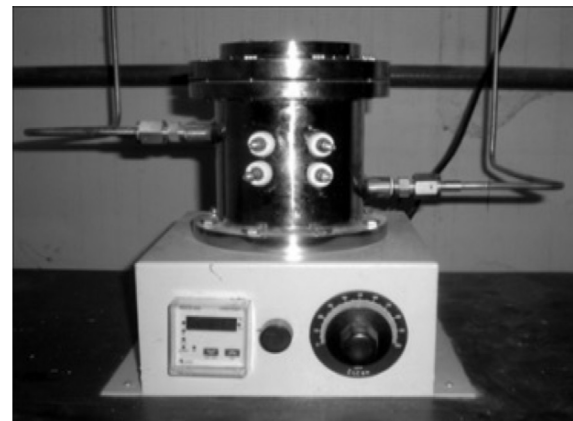
Intelligent recognizer for the component analysis of toxic mixture of (sewer) gases



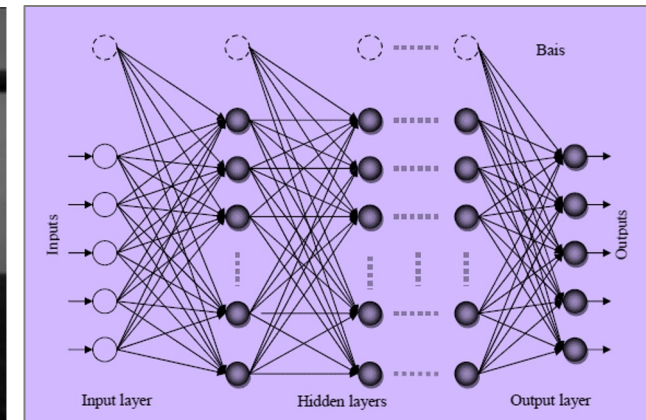
Gas mixture collection



Sensor array formation



Data collection and simulation

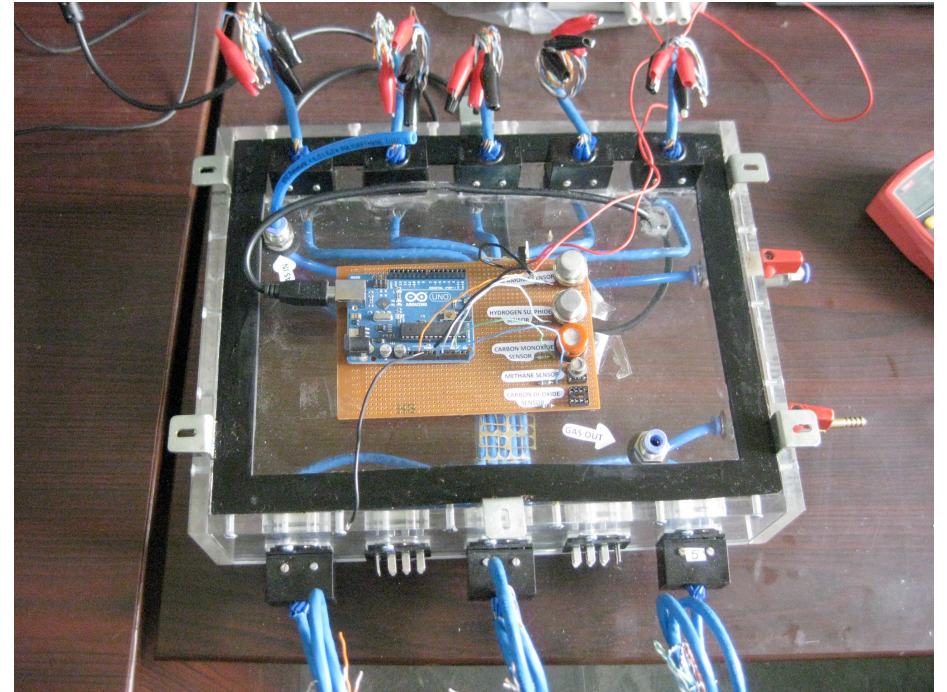


Pattern Recognition

Prototype of Intelligence Sensor



This was the objective
😊



We managed to get this one
nonetheless! (2011-2013)

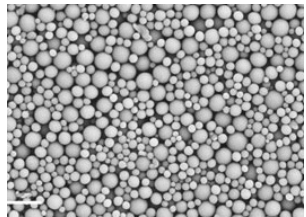
Pharmaceutical

Drug manufacturing process variables and
drug property analysis

Pharmaceutical (Drugs Production)



Pharmaceutical



Particle Properties
(Material type, density, size, shape and etc.)



Powder Properties
(Flowability, compactibility) +
(Roller gap and roller speed)



Ribbon Properties
(Density, Hardness, Porosity) + (Milling speed etc.)



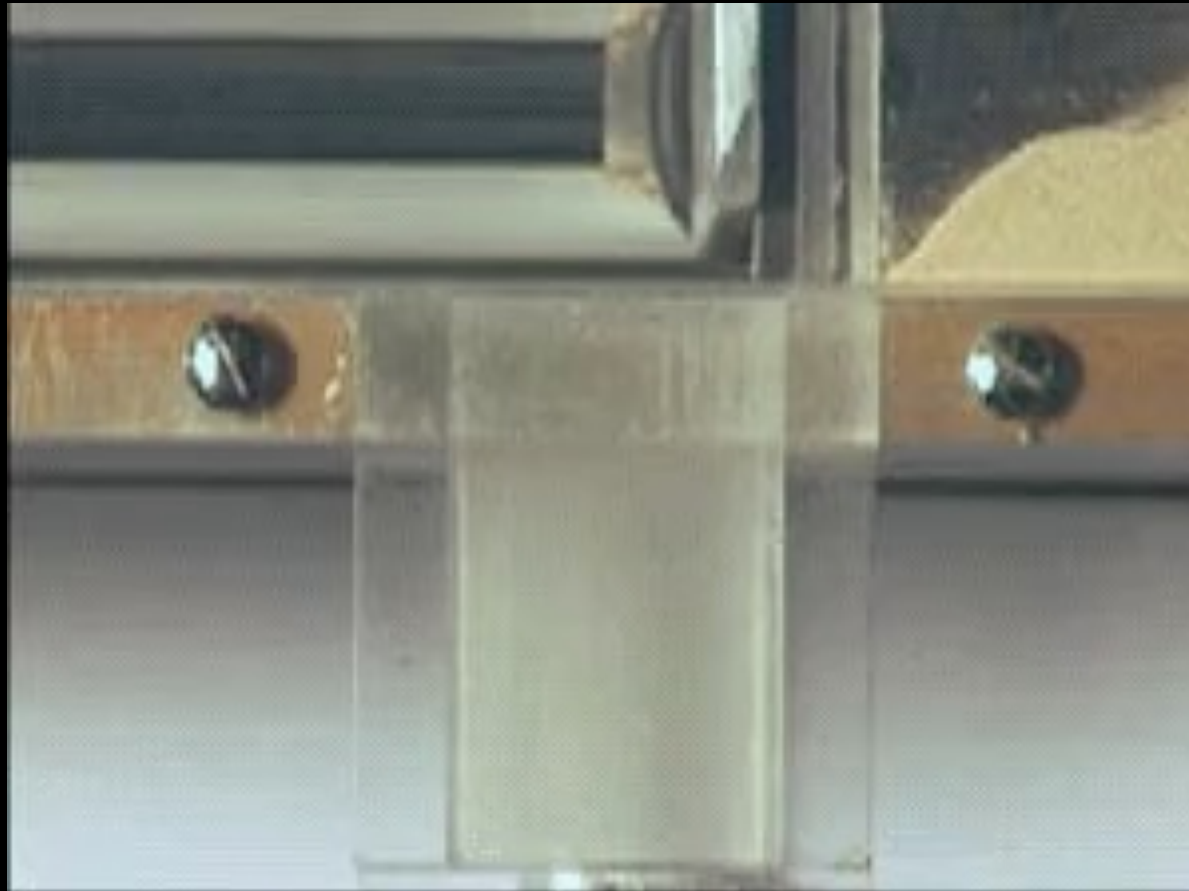
Granule Size Distribution + (die filling process)



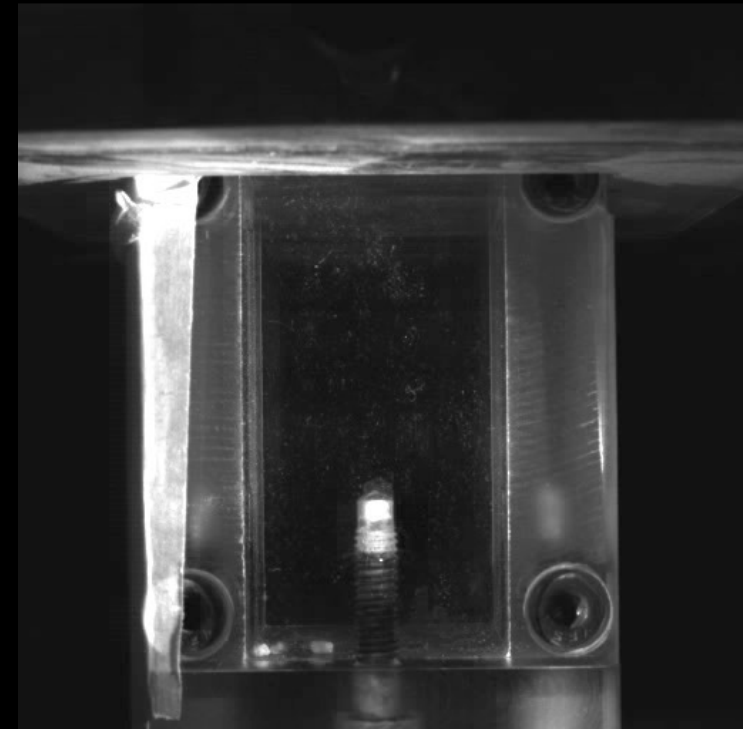
Tablet Properties
(Compressibility)

Variable Identification of Pharmaceutical Industrial Processes

Prediction of the mass of deposited drug powder



Photron FASTCAM SA4 mode...
1000 fps 1/1000 sec 512 x 512
End frame : -1150 -1150 ms
Date : 2015/1/14 Time : 19:41



Drug Dissolution

Ojha VK et al. (2015) International Journal of Nanomedicine



Three Hundred Descriptors of Drug Properties

PLGA: poly(lactic-co-glycolic acid)

SI No	Group name	No of features	Importance
1	Protein descriptors	85	Describes the type of molecules and proteins used
2	Formulation characteristics	17	Describe the molecular properties such as molecular weight, particle size, etc
3	Plasticizer	98	Describe the properties such as fluidity of the material used
4	Emulsifier	99	Describe the properties of stabilizing/increase the pharmaceutical product life
5	Time in days	1	Time taken to dissolve
6	% of molecules dissolved	1	Output

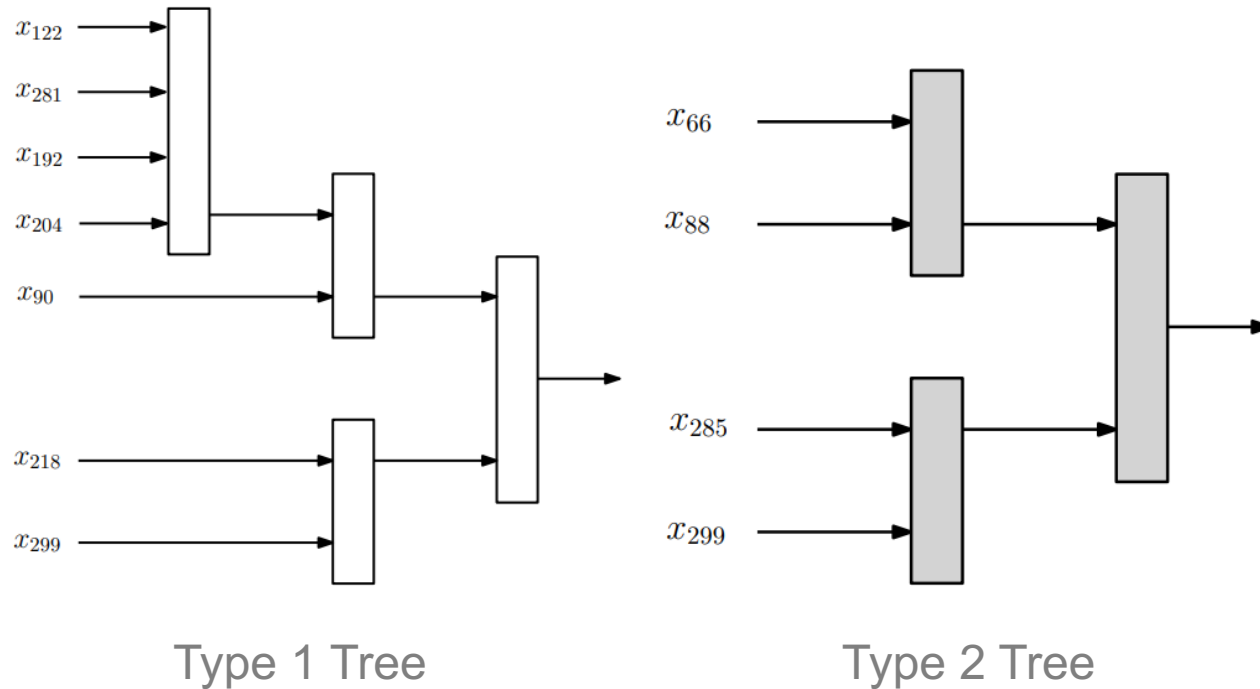
Abbreviations: PLGA, poly(lactic-co-glycolic acid); SI, serial; No, number.

Balancing Prediction and Feature Selection

Algorithm	RMSE E_t	No. of features
MLP	14.3	17
Neural Tree	13.2	15
REP Tree	13.3	15
GPR	14.9	15
MLP	15.2	15
MLP	15.4	11
Type 1 Tree	18.6	7
Type 2 Tree	15.2	4

A Tree Model for Future Use

Can we also explain how the prediction was made?



If protein is **A** and plasticizer is **B**, **Then** % molecule dissolution is **X**

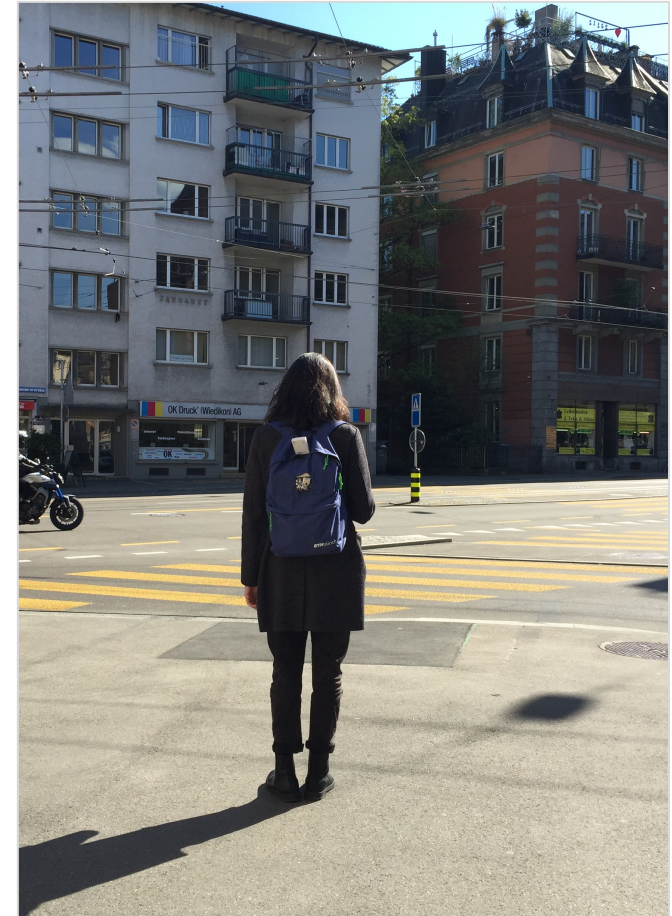
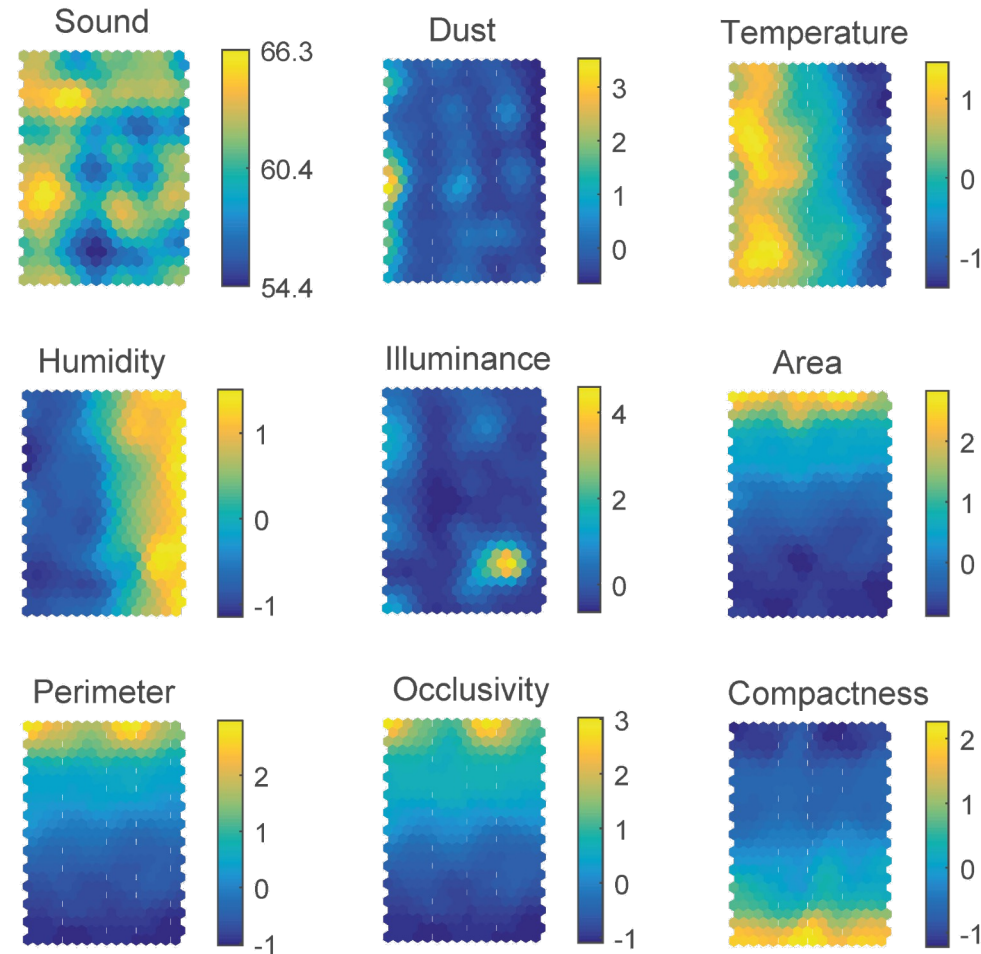
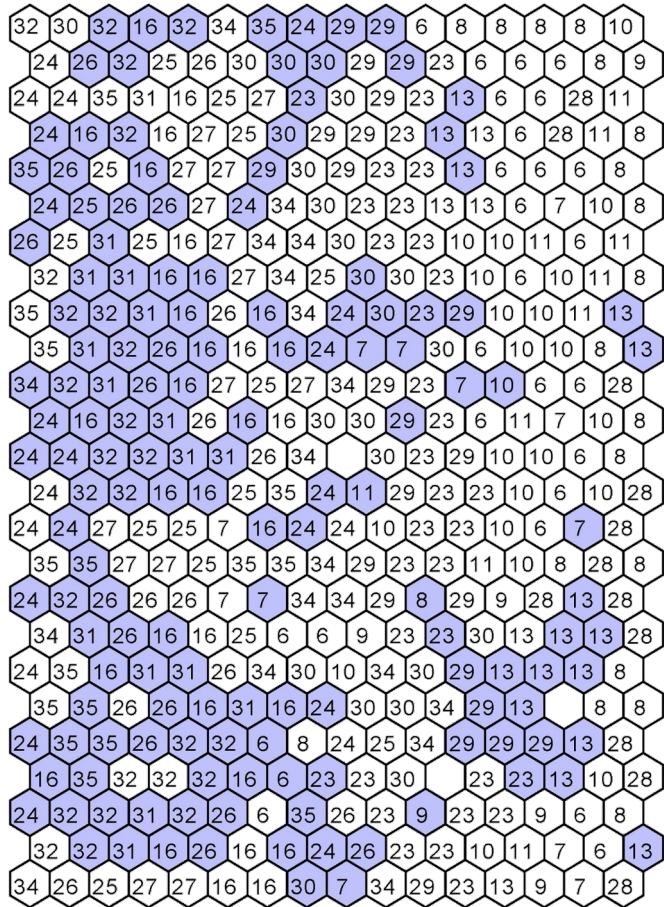
Build Environment

Understanding impact of environment and urban
dynamics on humans

Perception of the Environment



Perceptual Experience



Civil Engineering

Structure buckling analysis

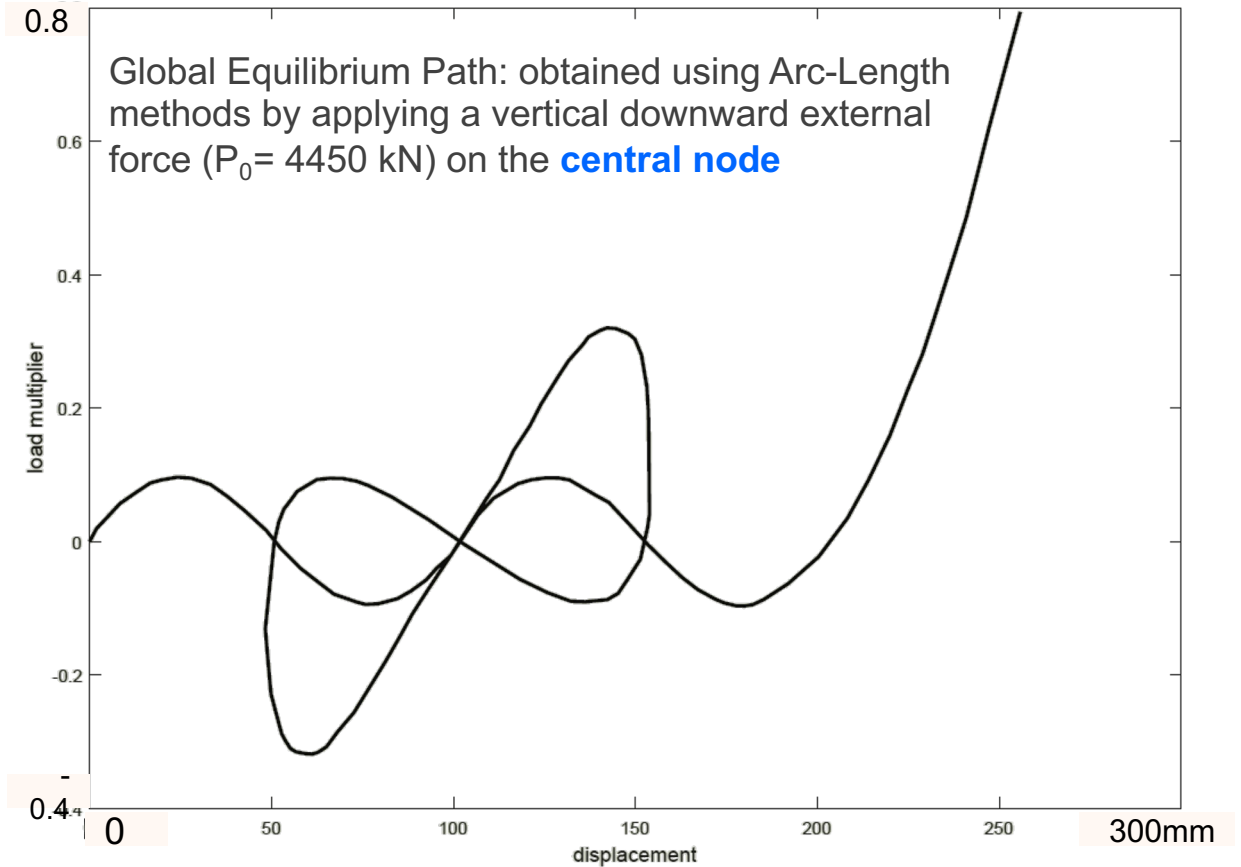
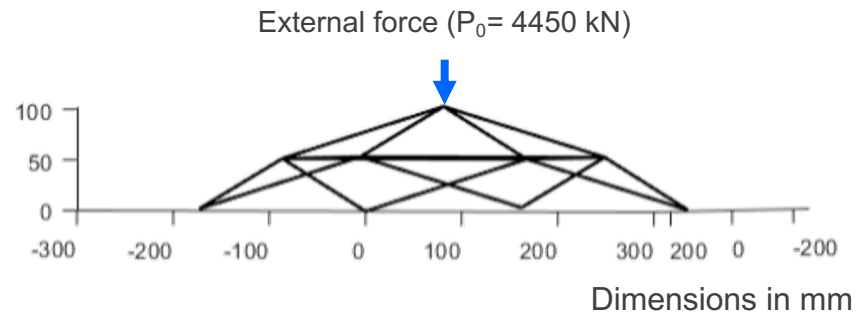
Civil Engineering Problem



Civil Engineering Problem



A tiny version of Millennium Dome can be the following structure



Hrinda, G. (2010, April). Snap-through instability patterns in truss structures. In 51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference 18th AIAA/ASME/AHS Adaptive Structures Conference 12th (p. 2611).

Civil Engineering Problem

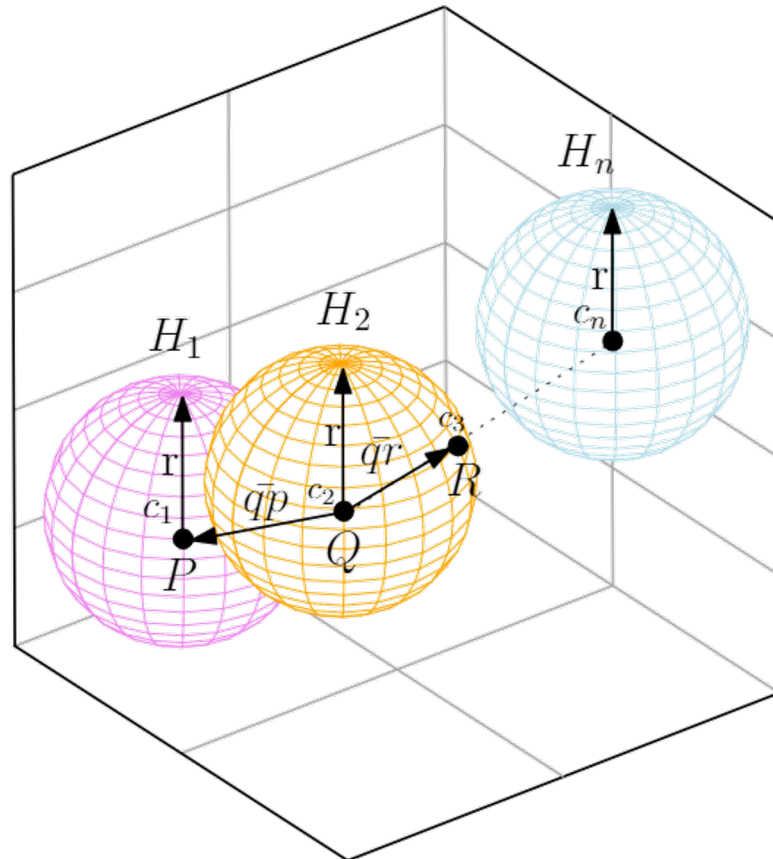


Fig A. Adaptive Hypersphere Search Algorithm for Structural Static Analysis

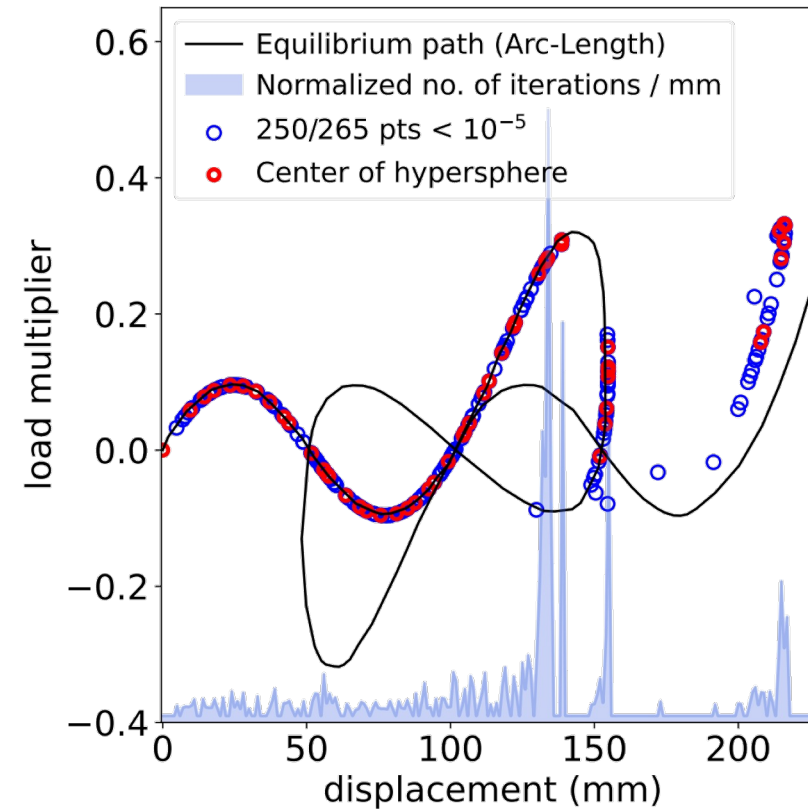
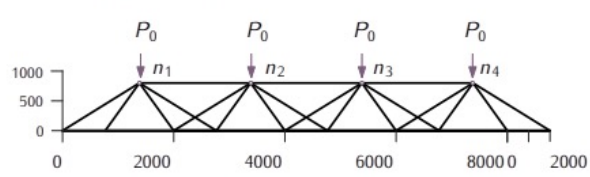


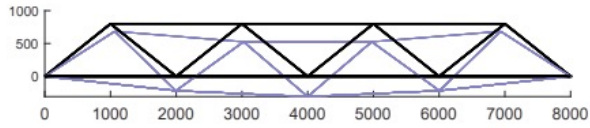
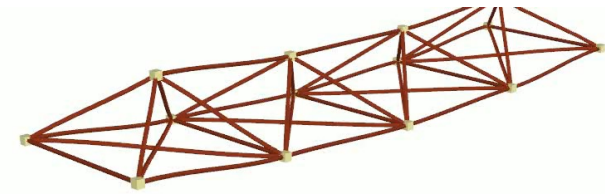
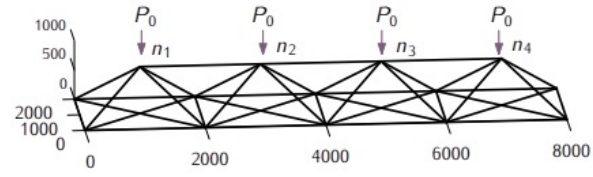
Fig B. Equilibrium Path traced using Adaptive Hypersphere Search Algorithm

Side view (2D view)

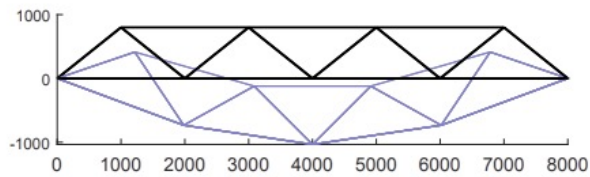
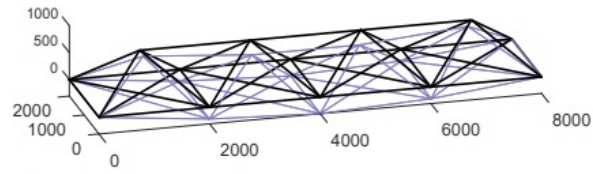


Undeformed shape

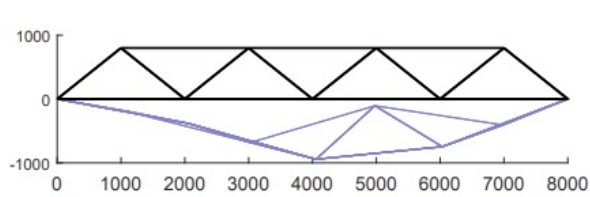
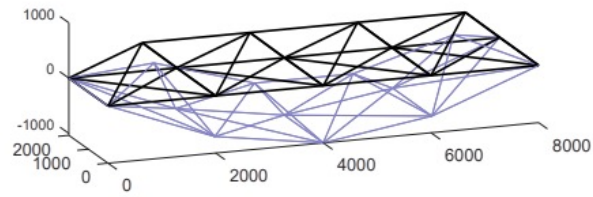
Top view (3D view)



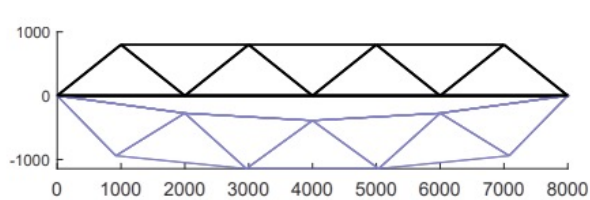
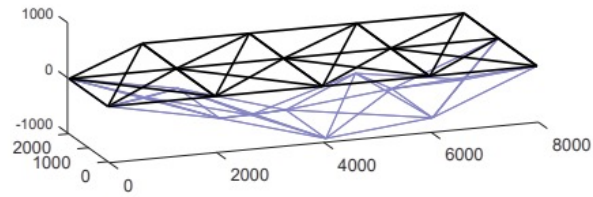
Deformed shape A



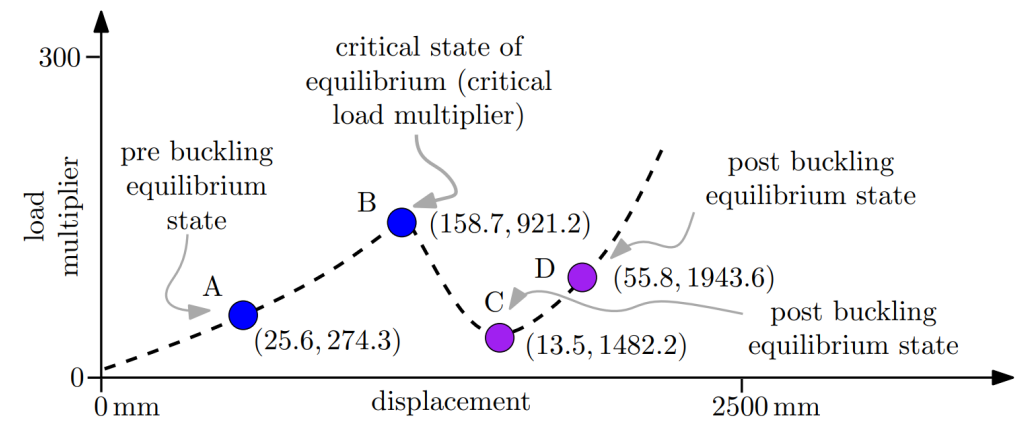
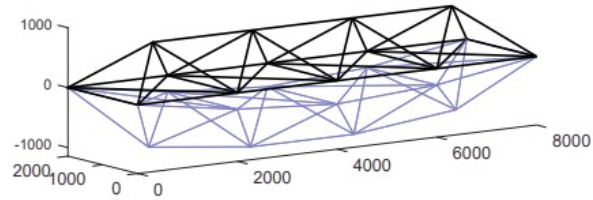
Deformed shape B



Deformed shape C



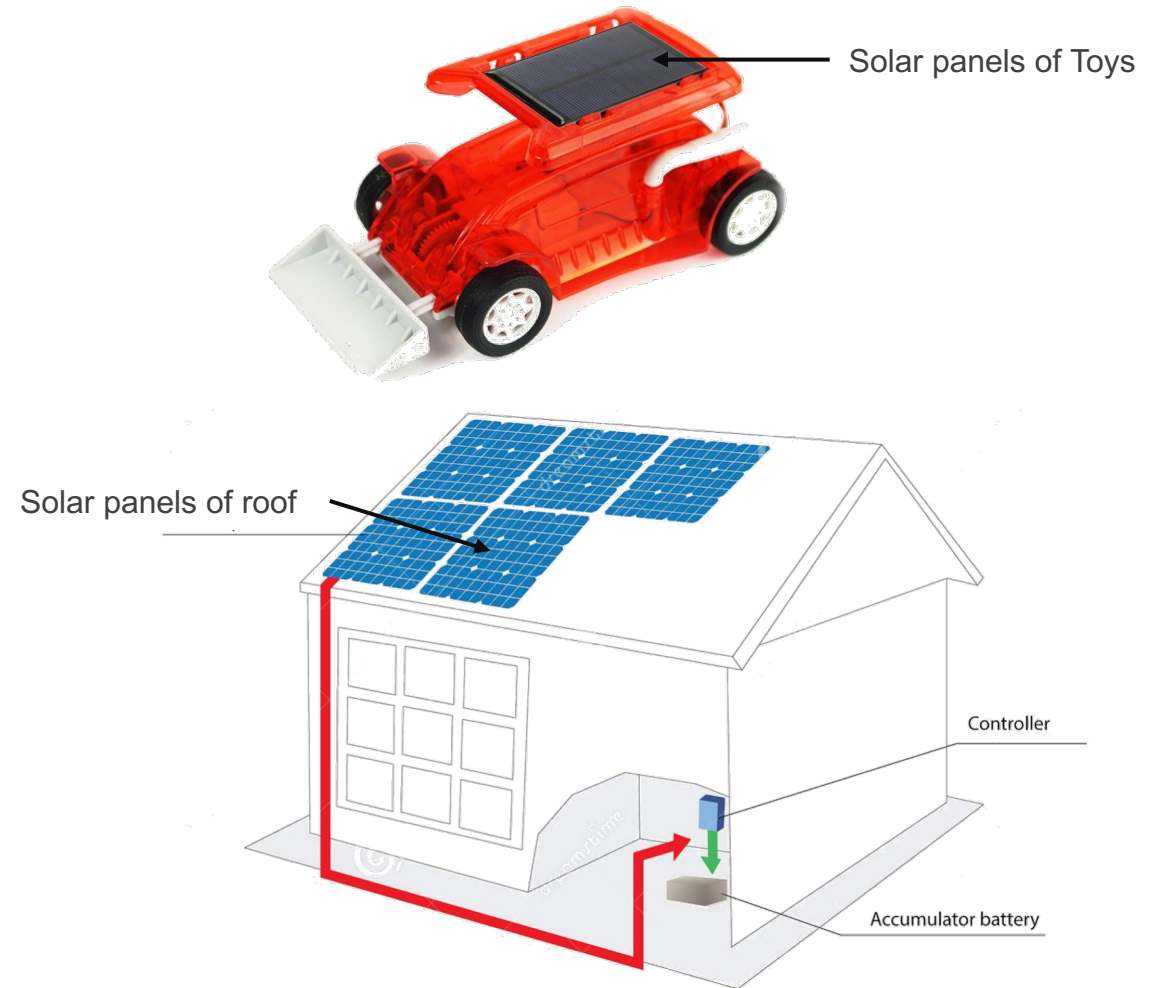
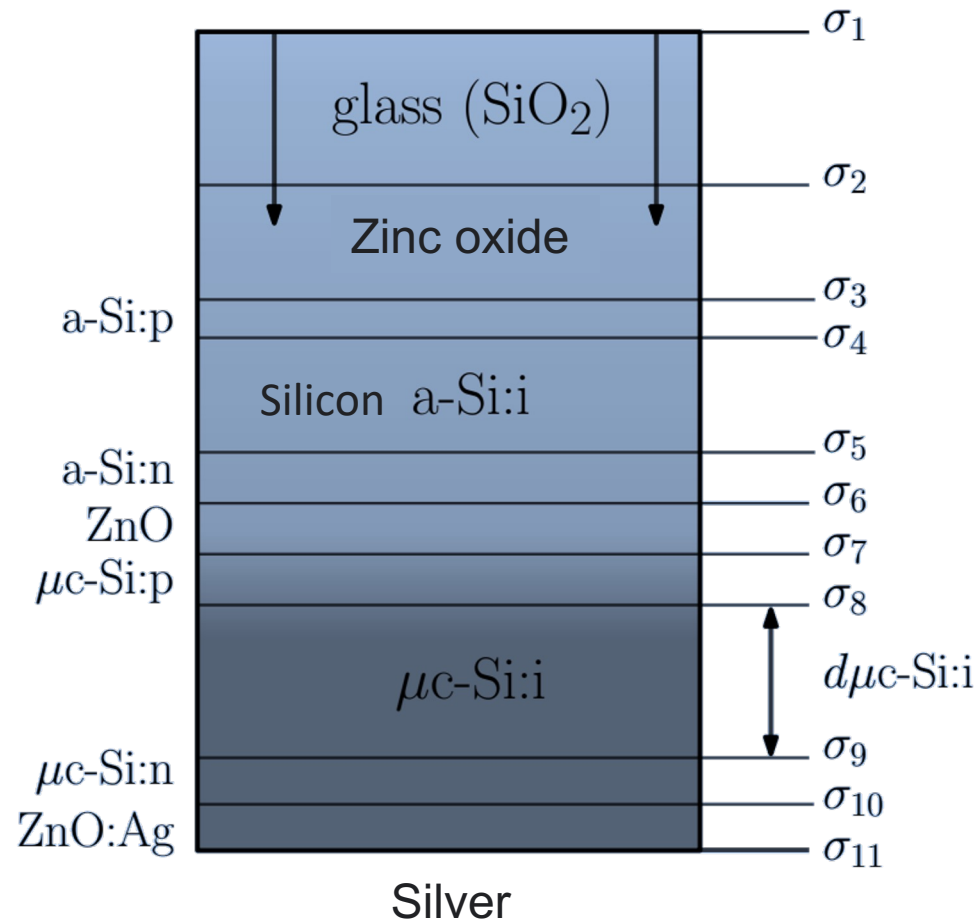
Deformed shape D



Physics

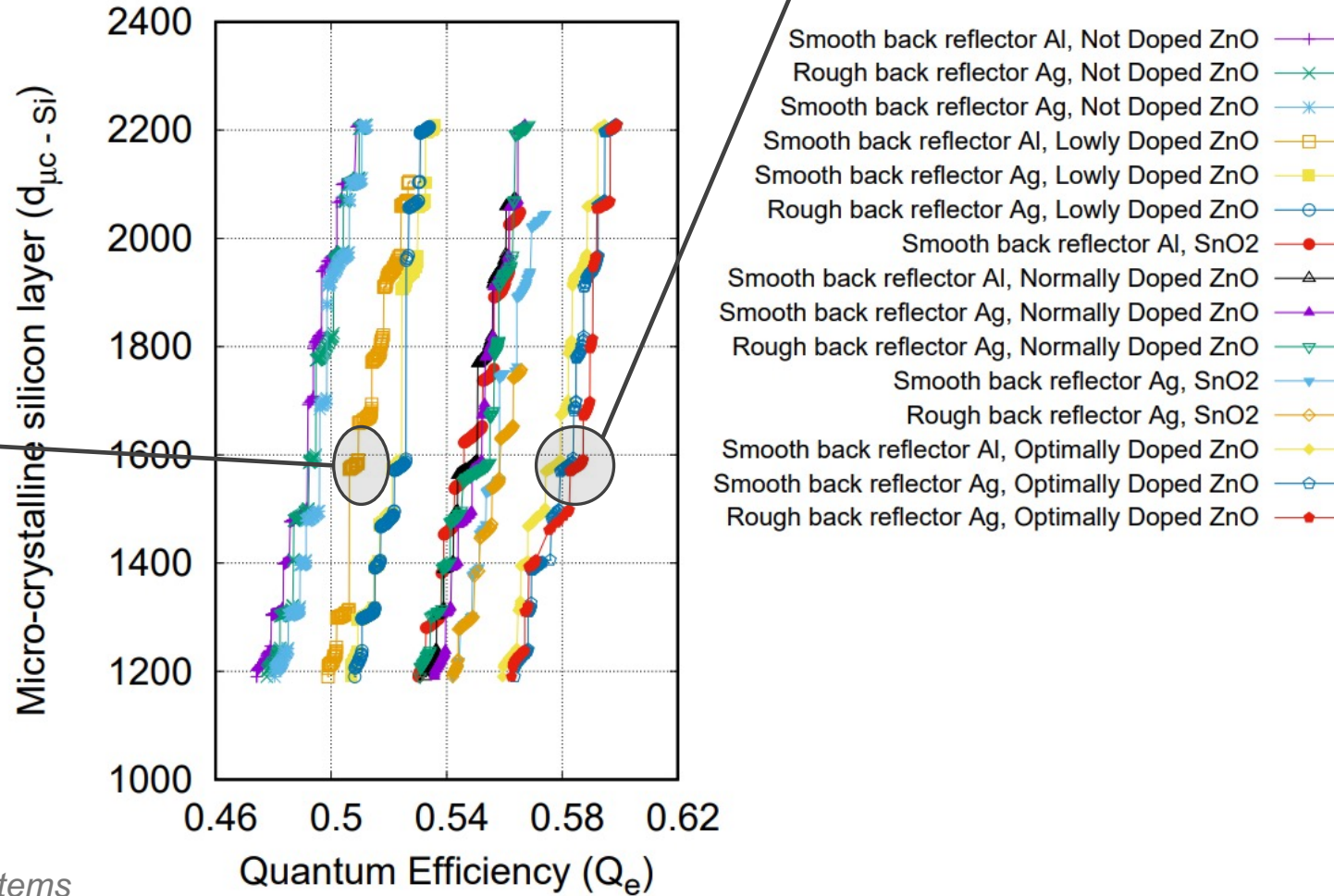
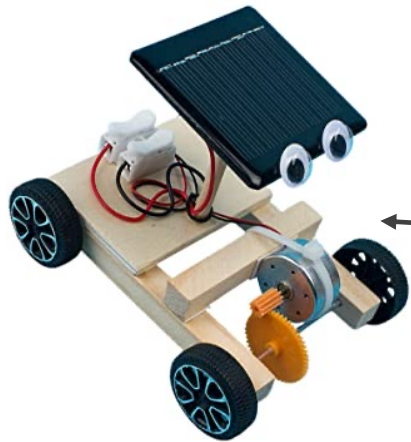
Solar cell design and characterization

Solar Cell – Energy Optimization



Solar Cell

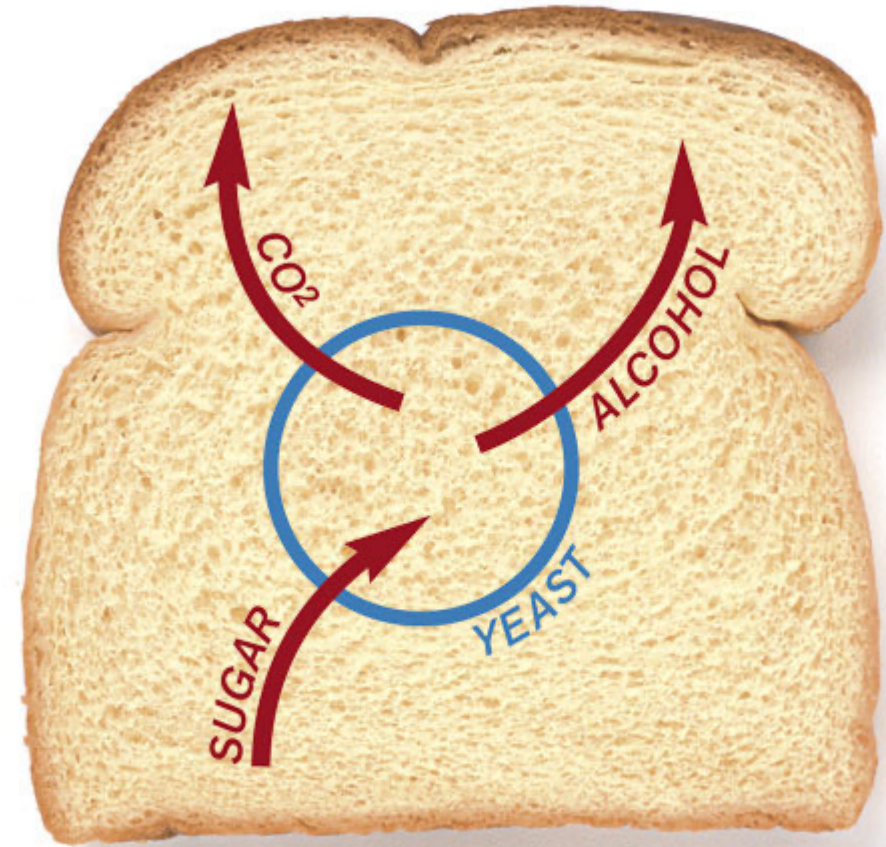
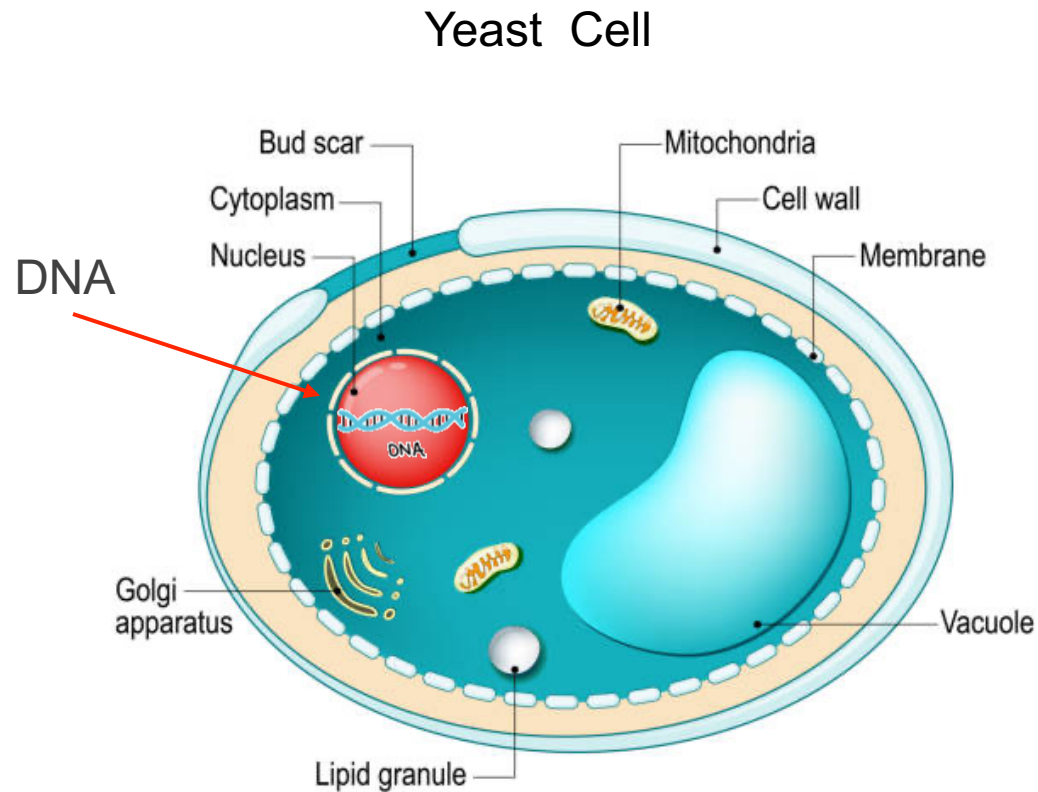
Cost and Efficiency Trade-offs for its Usage

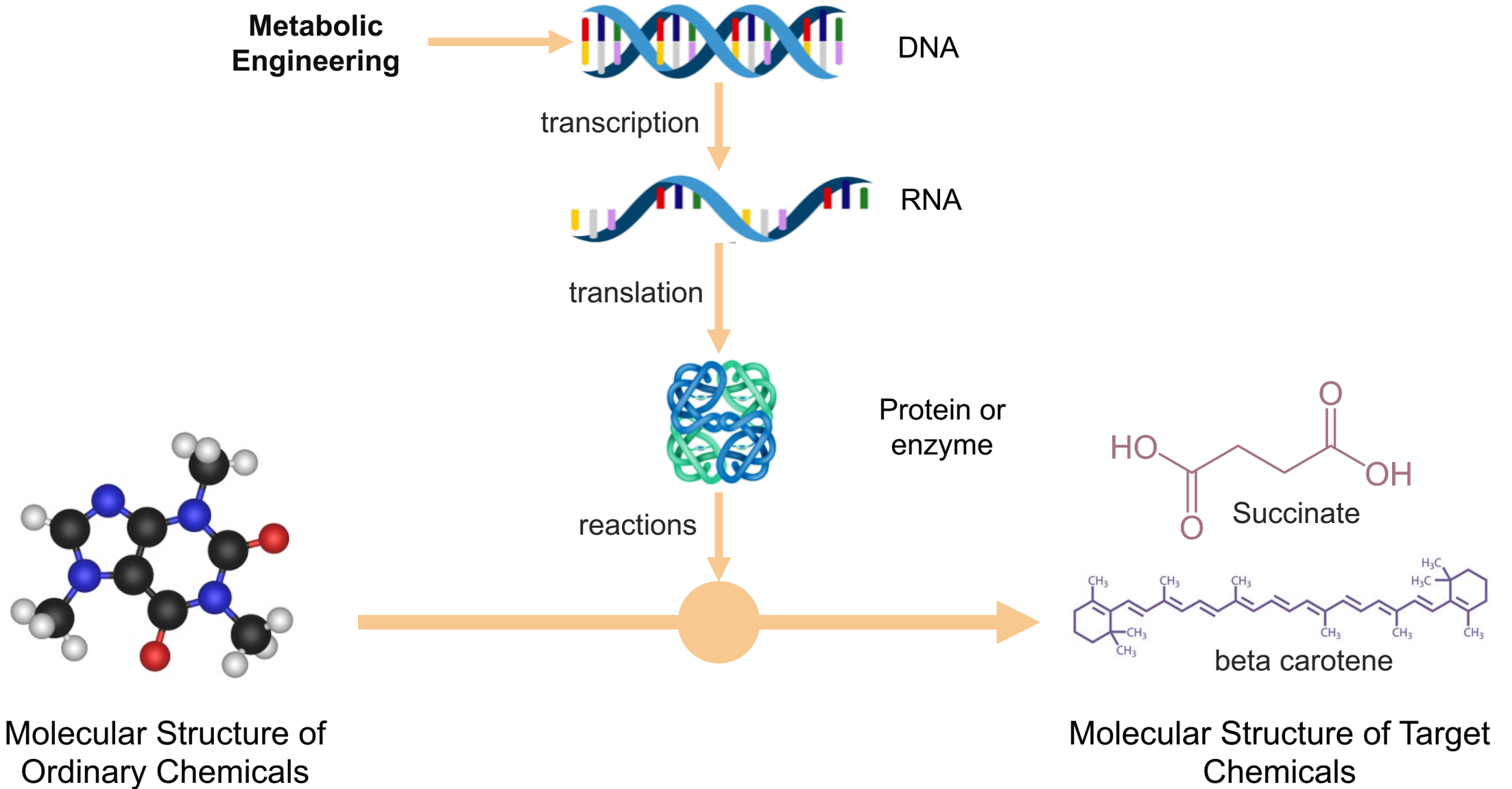


Biology

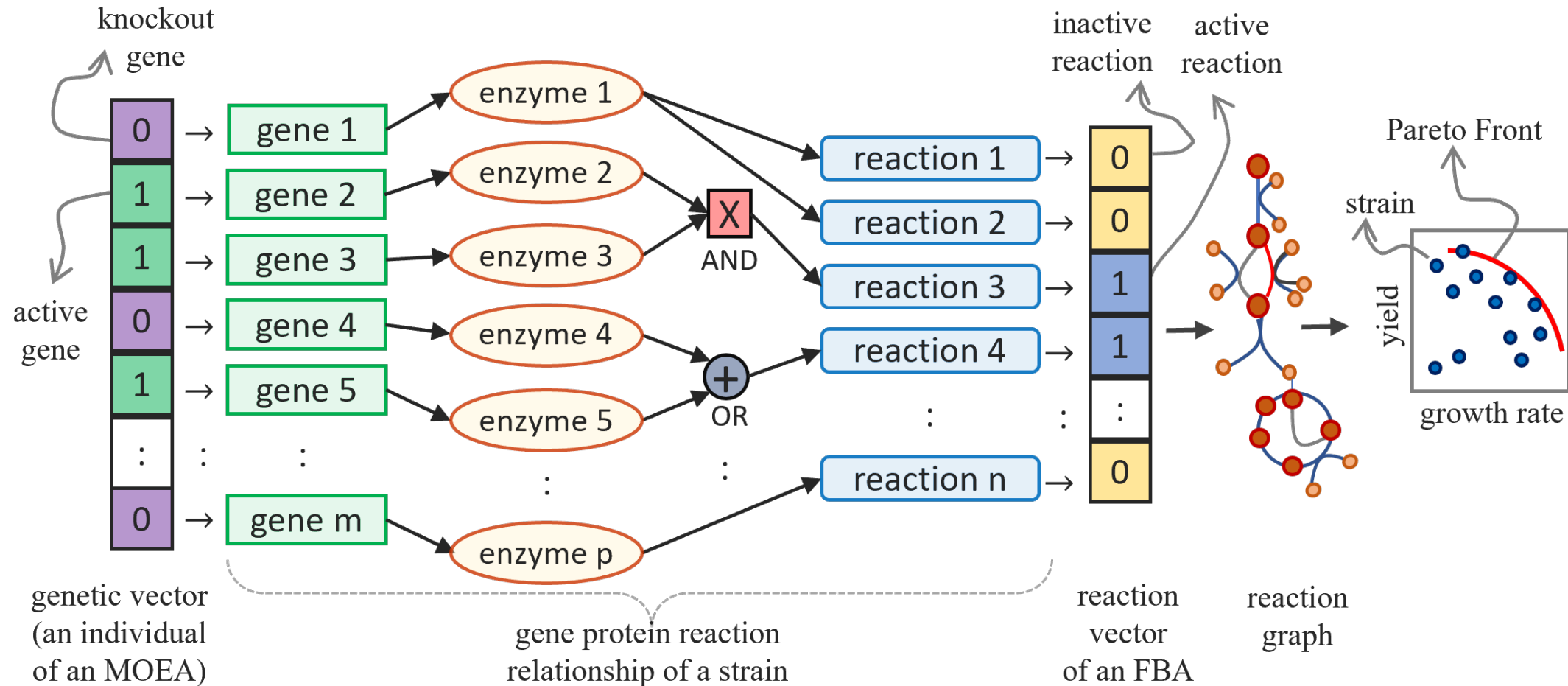
Metabolic engineering (searching for best strains)

Role of Yeasts in Food Production

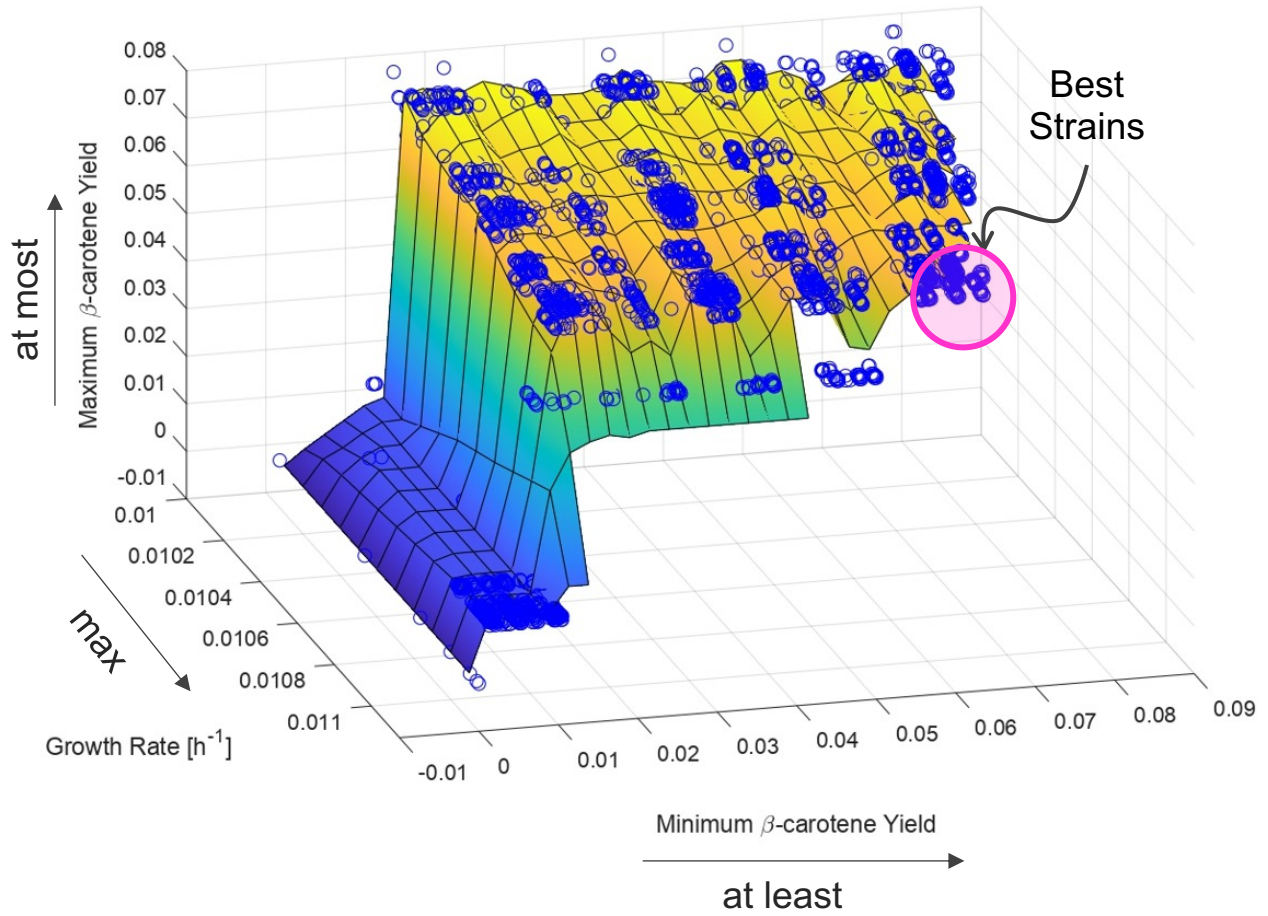
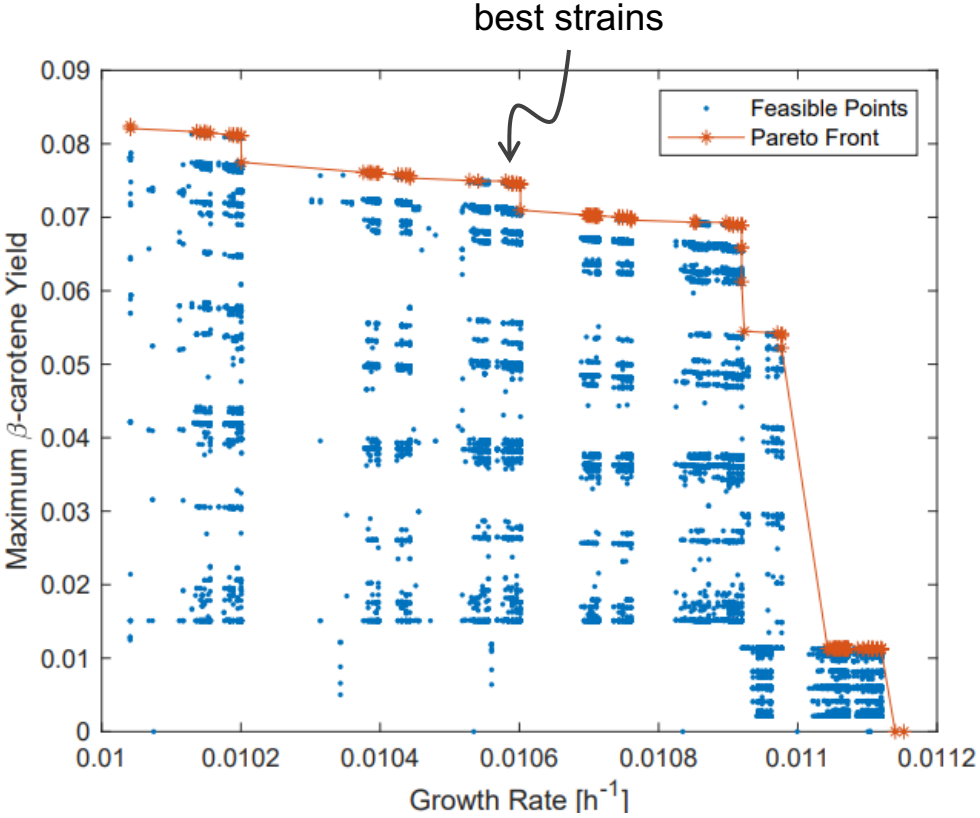




Metabolic Engineering for Chemical Production



Optimal Strains of Yeast



Hydrology

Prediction of flood events

Hydrology: Flood Event Prediction

A collaboration with Meteorology (Prof. Sarah Dance and Remy Vandaele)

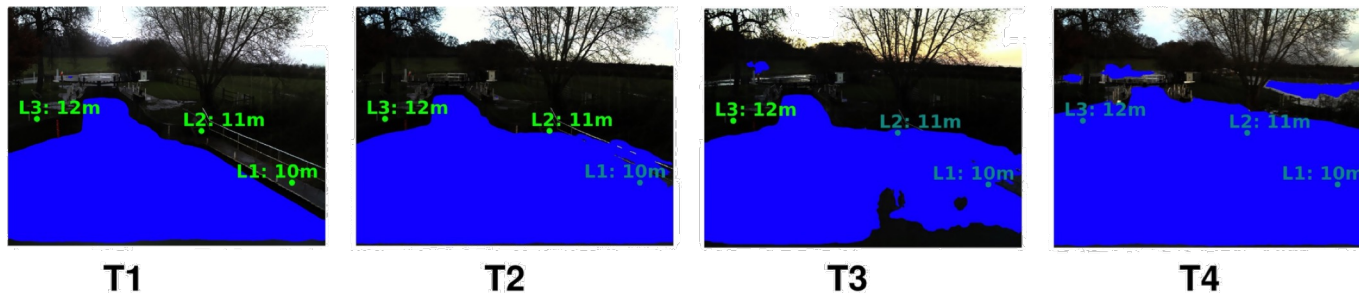


Fig. Time-series sequence of images of river. Blue pixels are water segmentation by using deep learning models



Credit: Farson Digital Watercams
https://www.farsondigitalwatercams.com/locations/keswick_greta

Hydrology: Flood Event Prediction

A collaboration with Meteorology (Prof. Sarah Dance and Remy Vandaele)

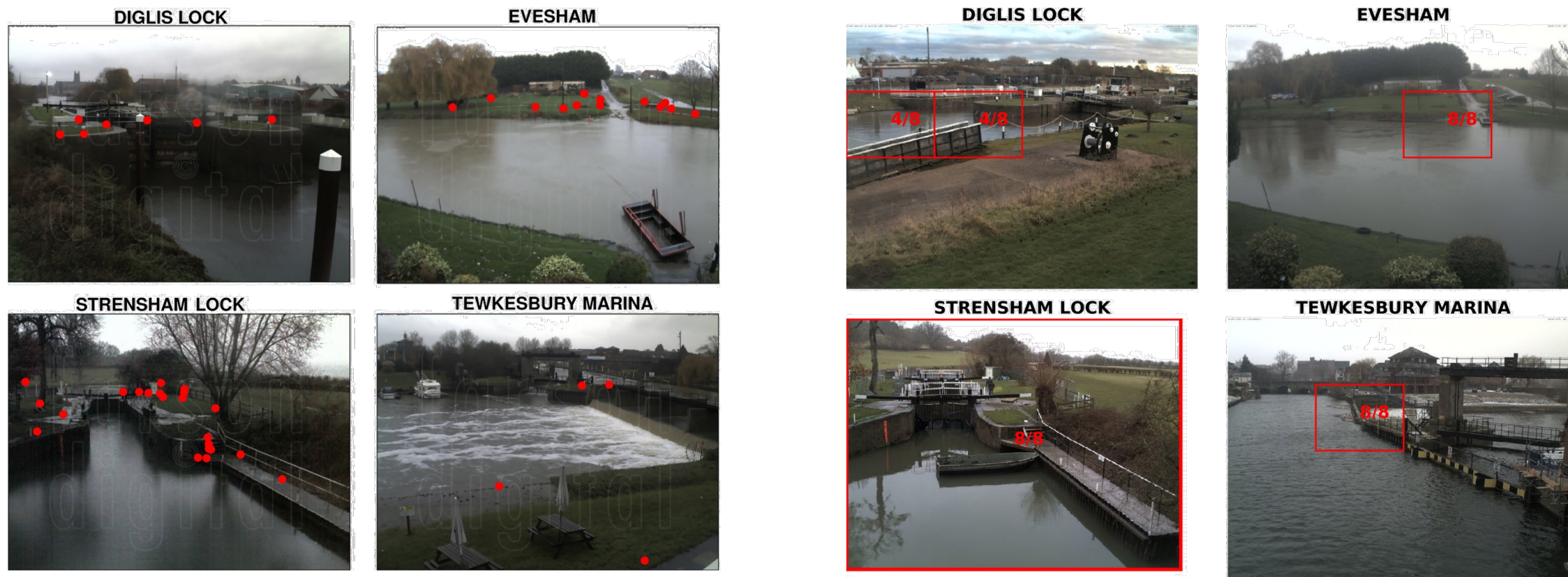


Fig A. Customized dataset:

Landmark annotation of waterline

Vandaele, Dance, and Ojha, (2021) *Hydrology and Earth System Sciences*

<https://doi.org/10.5194/hess-25-4435-2021>

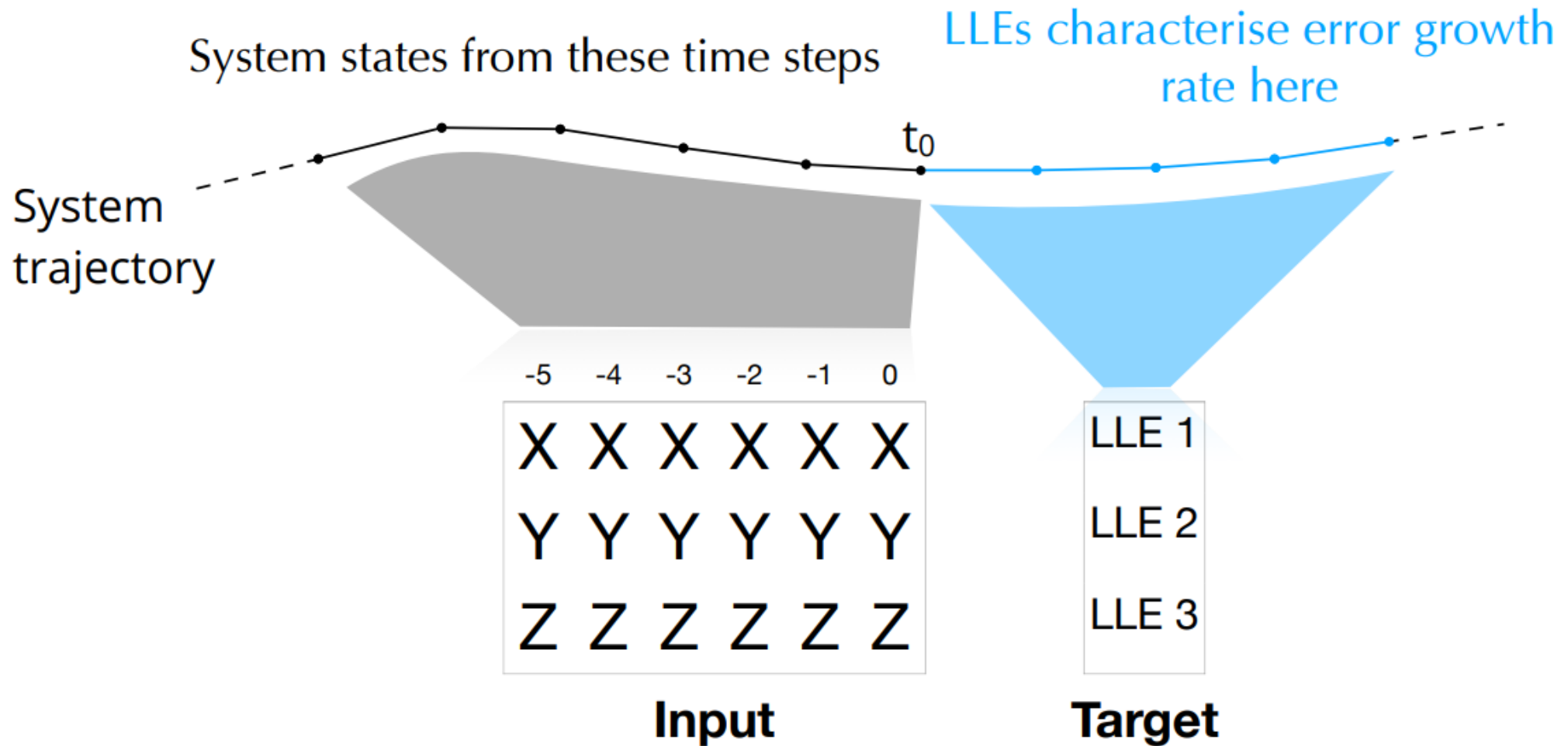
Fig B. Best window identification for prediction accuracy.

We achieve 94% accuracy in correctly predicting real flood events.

Climate Science

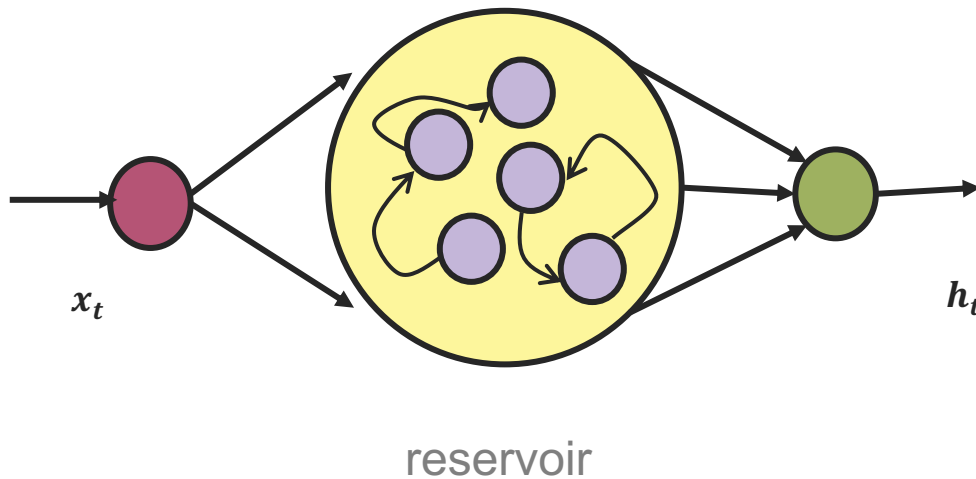
Non-intrusive modelling of dynamical systems

Predicting Instabilities in Chaotic Systems

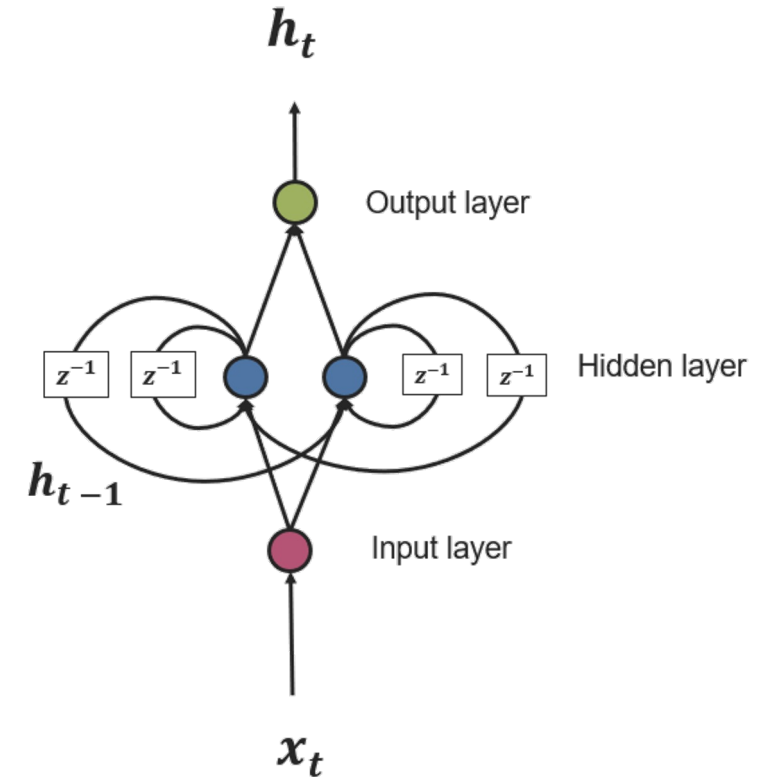


Machine Learning Algorithms to Use

Supervised **recurrent neural networks** for the reconstruction short term dynamics



Eco State
Network



Long Sort Term
Memory

What LOSS function can we use?

We can consider two types of losses:

- **Purely Data Driven loss (Neural Nets):**

- $loss = \frac{1}{N} \sum (x_{t+1} - f(x_t))^2$

- **Physics Informed loss (Physics Informed Neural Nets)**

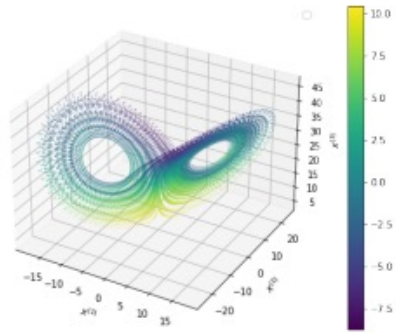
- $loss = \frac{1}{N} \sum (x_{t+1} - f(x_t))^2 + \text{physics (e.g., } |RK_4(x_t) - RK_4(f(x_t))|)$

Data Driven Neural Nets

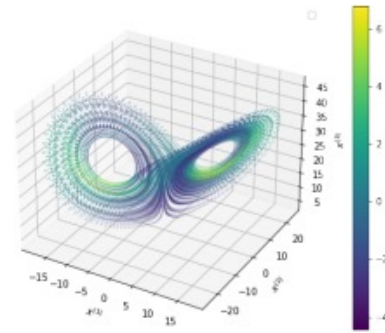
(prediction of short term dynamics)

Rössler 76 Lorenz 63

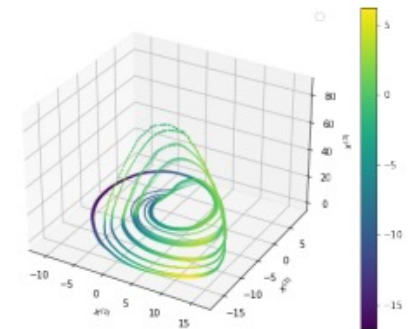
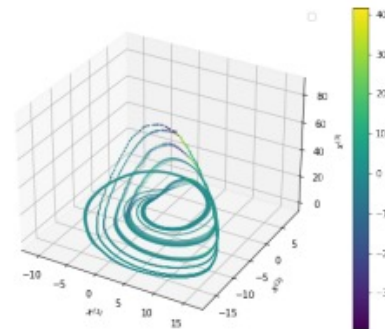
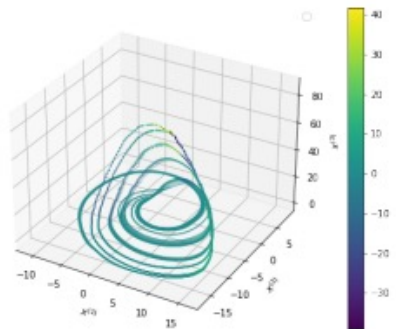
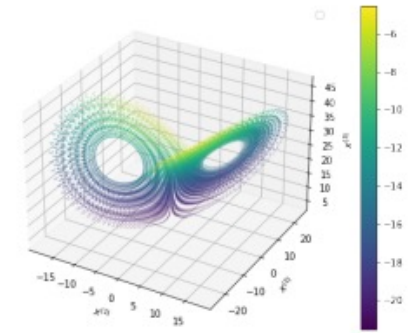
LLE1



LLE2



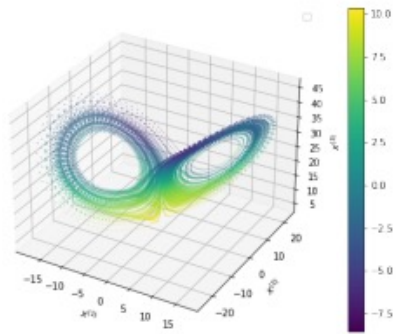
LLE3



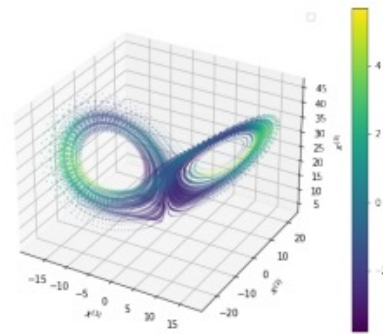
Physics Informed Neural Nets

(prediction of short term dynamics)

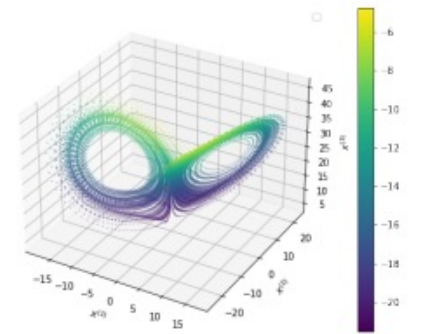
LLE1



LLE2

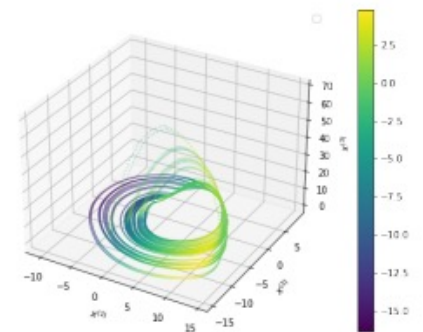
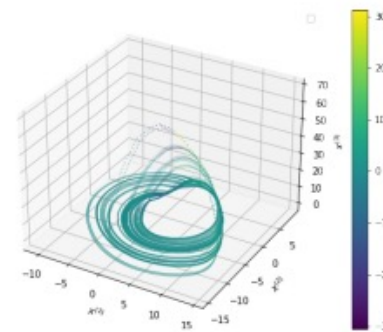
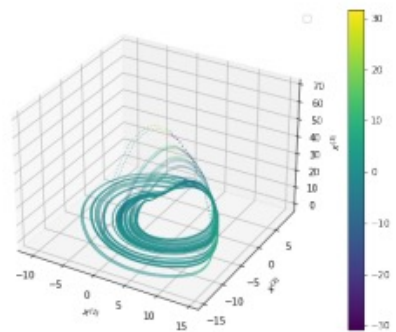


LLE3

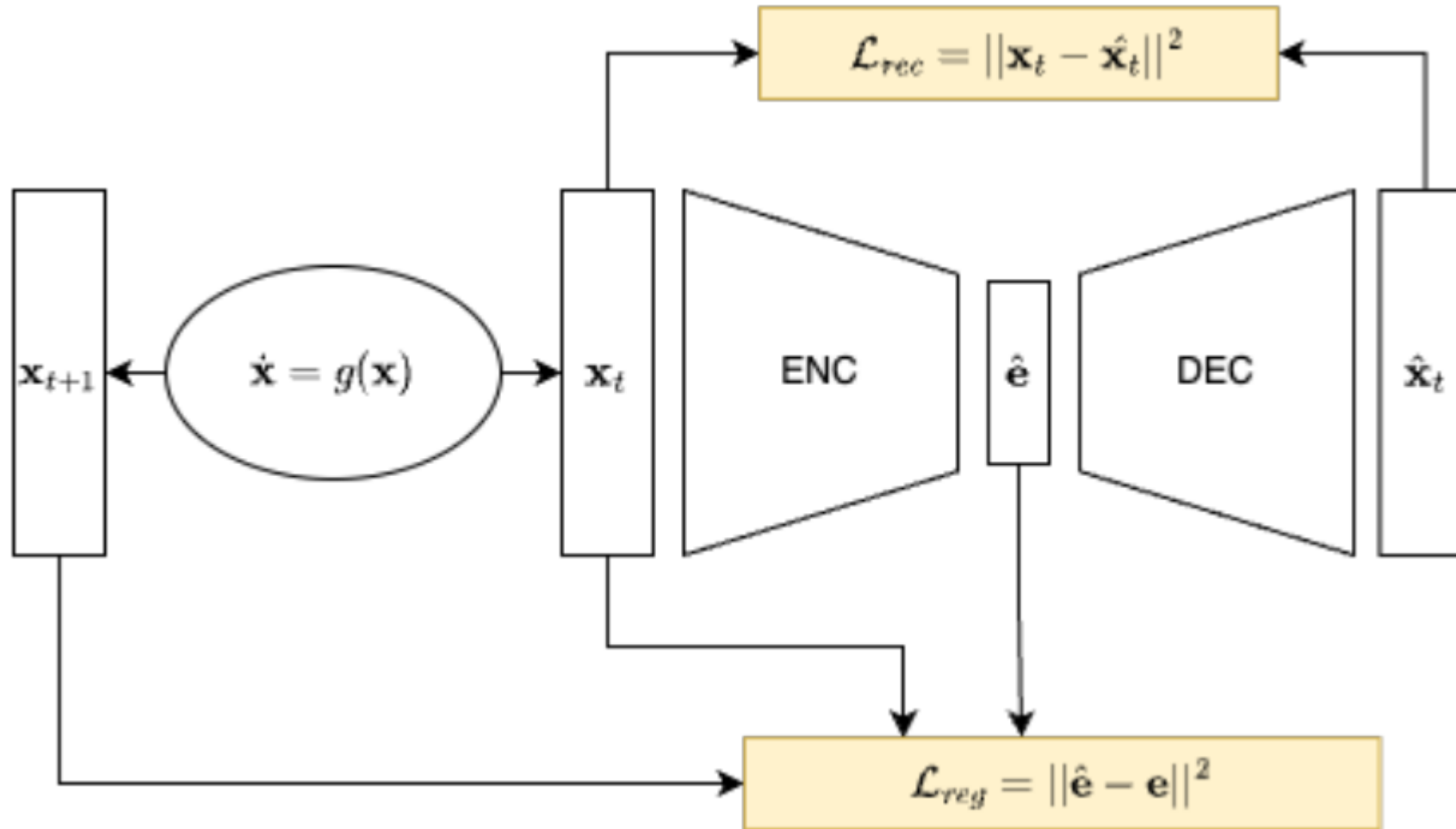


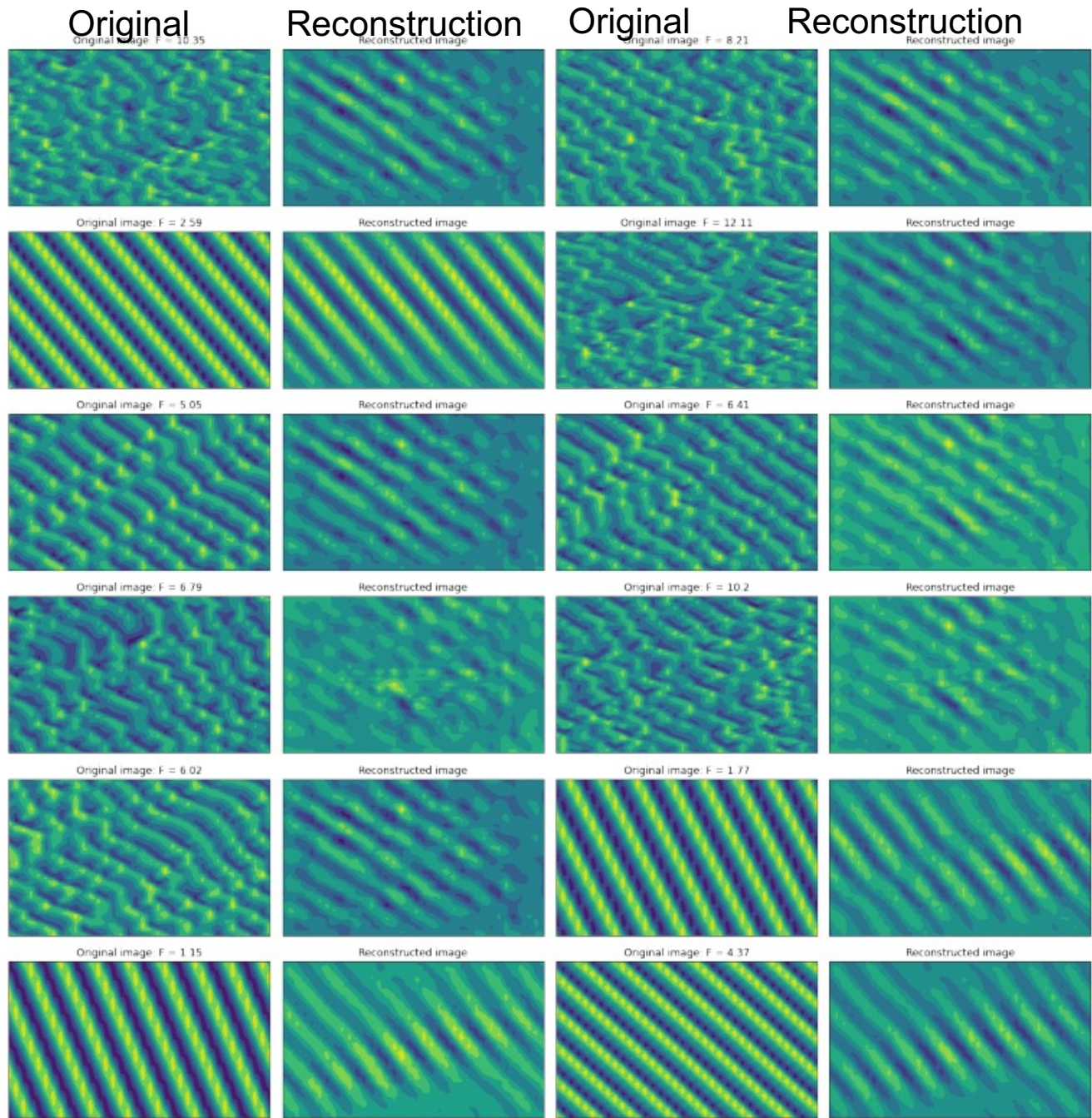
Rössler 63

Rössler 76



Symmetric Convolutional Autoencoder





Plastic Waste Pollution (Input Video)



AI Solution (Output Video)



Jaikumar P et al. (2020) ISDA, <https://centaur.reading.ac.uk/98569/>

v.k.ojha@reading.ac.uk