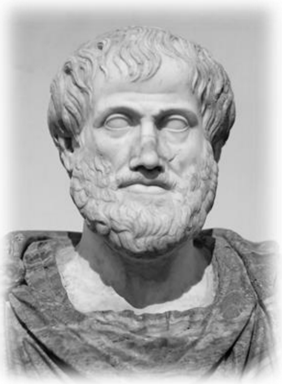
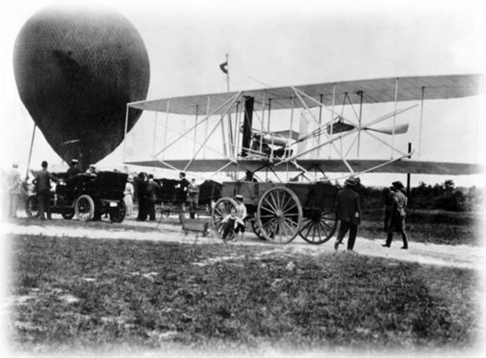
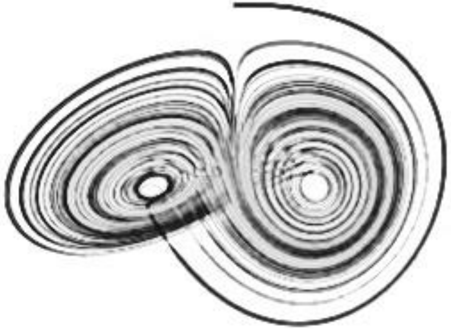
Data Driven Engineering I: Machine Learning for Dynamical Systems

Basics I: Introduction to DDE

Institute of Thermal Turbomachinery
Prof. Dr.-Ing. Hans-Jörg Bauer



Today’s Agenda

i. Flow of the Lecture

ii. A holistic view on AI and ML

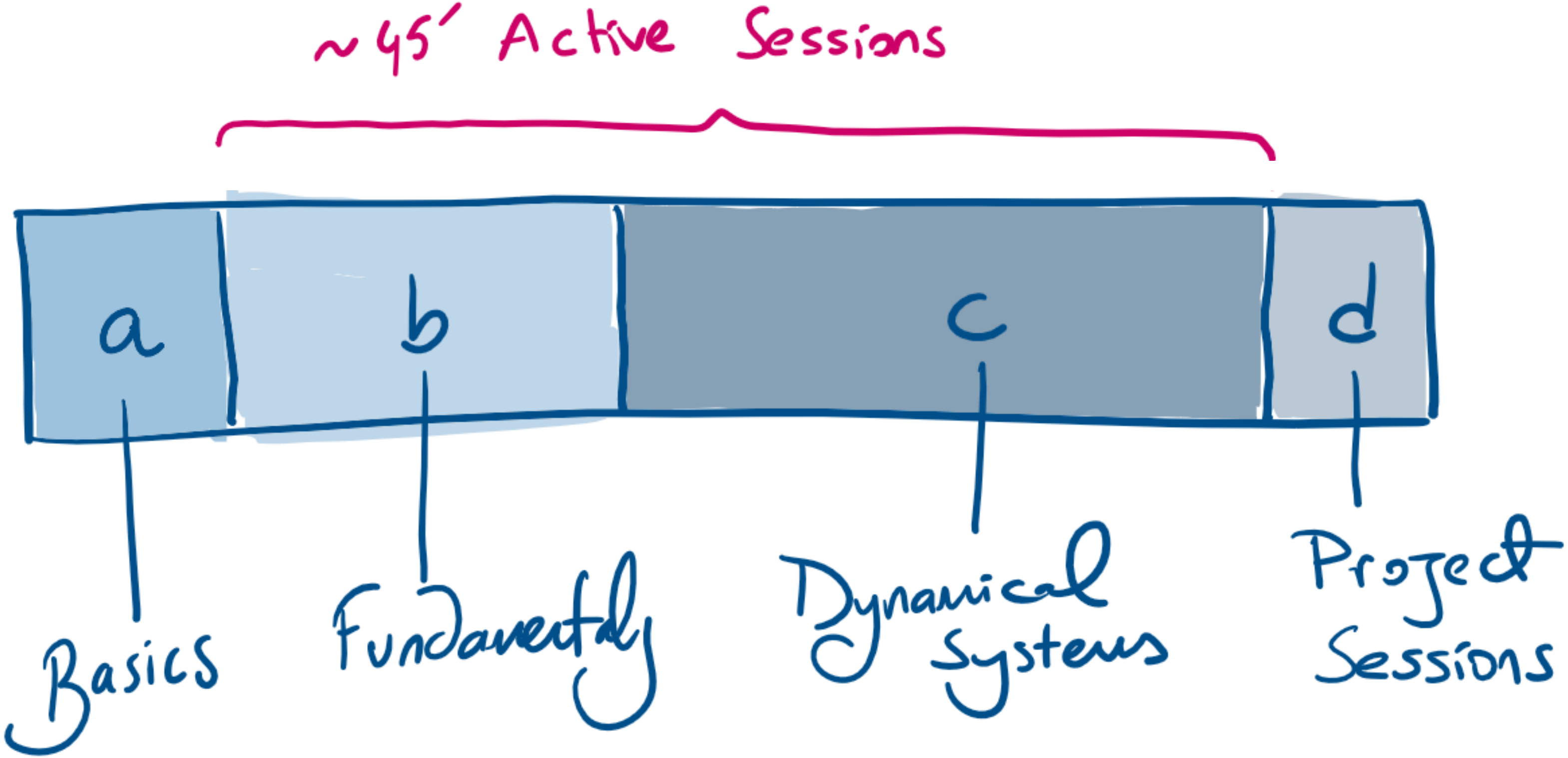
iii. Data Driven Engineering

iv. Recent Developments and Examples

The Style

DDE II Advanced Topics

DDE 1 Curriculum



Active Sessions

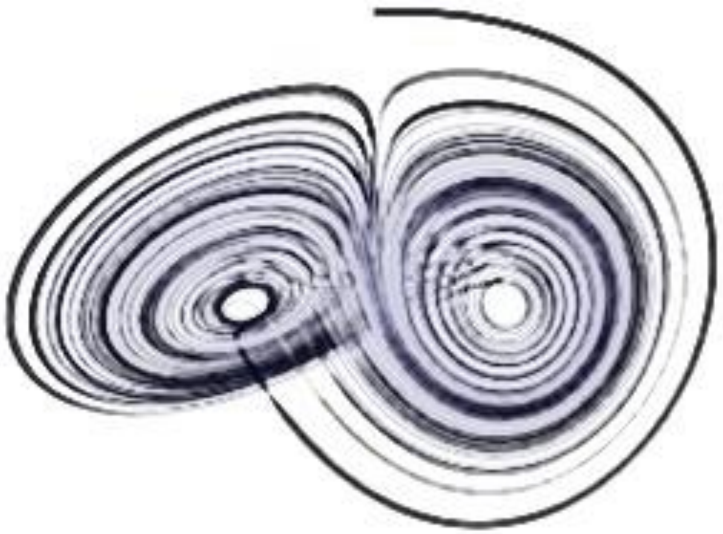
- ❑ Colaboratory, or "Colab" for short, allows you to write and execute Python in your browser
- ✓ Zero configuration required
- ✓ Free access to GPUs (limited)
- ✓ Easy sharing and file management
- ○ You need a google account (dummy) // Local installation on PC

Projects & Grading Policy

- End of semester: end-to-end ML project
- Individual tasks: unique datasets
- Dataset selection 1: Recommended list
  - ILIAS Forum
  - First comes, first served
- Dataset selection 2: Custom datasets
  - Sources: ILIAS Forum
  - Needs to be approved
- Grading: Oral Exam

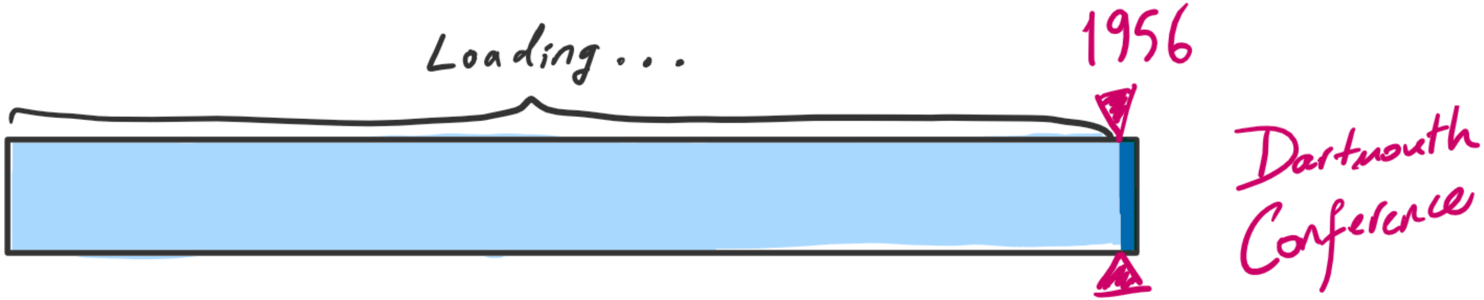
Datasets will be uploaded in two weeks

Deadline for selection: 24 / 12 / 2020



Data Driven Engineering: Machine Learning for Dynamical Systems

Birth of AI



Machines will be capable, within twenty years, of doing any work a man can do.

Herbert Simon, 1965

***

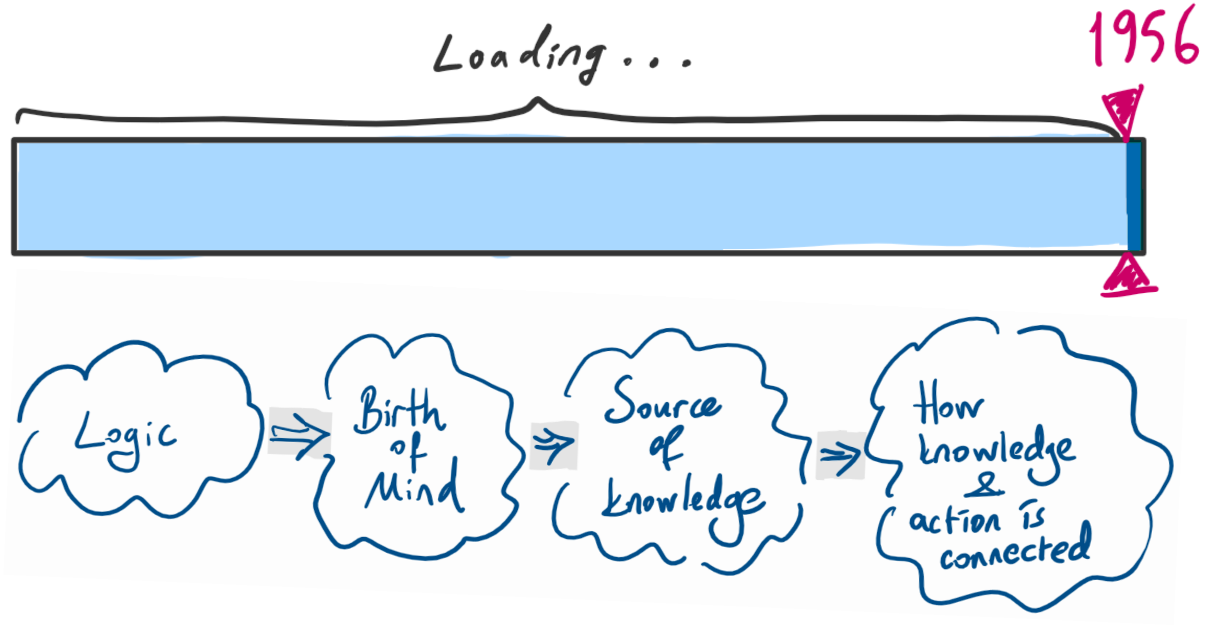
From three to eight years, we will have a machine with the general intelligence of an average human being.

Marvin Minsky, 1970

General AI ⇔ Machine Learning

General AI (Future)	Broad AI (Goal)	Narrow AI (1980s <)
• Cross-domain learning • Reasoning • Autonomy	• Multi-tasking • Transfer learning • Distributed sources • Explainable • Fair and unbiased • Small data	• Single task • Single domain • Knowledge based

Towards the Birth of AI and ML

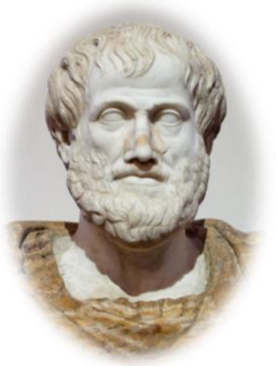


Interpreting the Intelligence: Logic

Rational thinking:

- Computational models
- Mental faculties
- Laws of thought

All men are mortal.
Socrates is a man.
Therefore, Socrates is mortal.



Aristotle
“Organon”

- Syllogism: **deductive reasoning** to arrive at a conclusion
- Logicist tradition within artificial intelligence
  - Informal => formal conversion
  - Uncertainity

Birth of Mind:Mechanical Artefacts

Foundations of AI
Philosophy
Mathematics
Economics
Biology
Psychology
Control Theory
Computer Eng.
Linguistics

- ✓ Ramon Llull (1300s):
  Pioneer of computation theory
- ✓ Lullian Circle: machine made of paper to combine elements of thinking
- ✓ “Reasoning could be achieved by a mechanical artefact”

Thomas Hobbes: “artificial animal,” (Leviathan 1651)
“For what is the heart but a spring; and the nerves, but so many strings; and the joints, but so many wheels.”

Birth of Mind:Mechanical Artefacts

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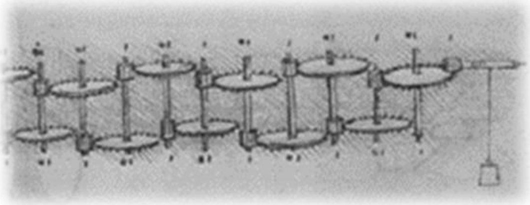

- ✓ Leonardo da Vinci: First mechanical calculator
- ✓ Wilhelm Schickard: Rechenuhr (1620)
- ✓ Pascaline of Pascal (1642)

  "Arithmetical machine produces effects which appear nearer to thought than all the actions of animals."

- ✓ Gottfried Wilhelm Leibniz (1694)

  "It is beneath the dignity of excellent men to waste their time in calculation when any peasant could do the work just as accurately with the aid of a machine."

Birth of Mind:as an entity

Foundations of AI
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Linguistics

✓ Dualism and Descartes (1600s)

distinction between mind and matter

✓ Materialism and Hobbes (1600s)

mental states and consciousness, are results of material interactions

Source of Knowledge

Foundations of AI
Philosophy
Mathematics
Economics
Biology
Psychology
Control Theory
Computer Eng.
Linguistics

If there is a physical mind that manipulates knowledge, what is the source of knowledge?

- ✓ Rationalism: Descartes, Spinoza, Leibniz (1600s)
  Reason is the source of knowledge
- ✓ Empiricism: Bacon, Locke, Hume (1600s, 1700s)
  "Nothing is in the understanding, which was not first in the senses."
- ✓ induction: Rules are acquired by exposure to repeated associations
- ✓ Logical positivism (1800s):= Rationalism + Empiricism

Connecting the knowledge and action

Foundations of AI
Philosophy
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Economics
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Linguistics

Action requires conclusion:
Conclusion := **logic** + computation + probability

✓ Logic: George Boole (1800s)
Laws of Thought (1854): Boolean algebra

✓ Logic: Gottlob Frege (1800s)
Exteneded to objects and relations
Created the first order logic

✓ Logic: Charles Sanders Peirce (1800s)
Deductive logic: “logical operations could be carried out by electrical switching circuits” (1886)

✓ Logic: Alfred Tarski (1900s)
Algebra of logic, and the theory of definability

“...universal laws of thought which are the basis of all reasoning,..., are at least mathematical as to their form.”
G. Boole

Connecting the knowledge and action

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Action requires conclusion:
Conclusion := logic + **computation** + probability

- ✓ Algorithm: Hârizmî (800s)
  Introduction of algorithmic recipes
- ✓ Algorithm: Boole and others (>1800s)
  Algorithms for logical deduction
  Mathematics of reasoning
- ✓ Computation: Gödel and others(1900s)
  Incompleteness theorem, Entscheidungsproblem
  Computability
  Tractability: time required grows exponentially with the size of the instances

Connecting the knowledge and action

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Action requires conclusion:
Conclusion := **logic** + **computation** + **probability**

- ✓ Fortune Telling ?
- ✓ Gambling: Mesopotamia 3000 BC
- ✓ Statistical inference: Middle East 700s, 800s

- ✓ Probability: Gerolamo Cardano (1500s)
  foundation of probability
- ✓ Probability: 1600s-1900s
  Pascal, Bernoulli, Laplace, Cotes, Legendre, Gauss
  Bayes, Bessel, Markov, Kolmogorov ...

Connecting the knowledge and action

- **Foundations of AI**
- **Philosophy**
- **Mathematics**
- **Economics**
- Biology
- Psychology
- Control Theory
- Computer Eng.
- Linguistics

Action requires conclusion:

Conclusion := **logic** + **computation** + **probability**

✓ Utility theory: Leon Walras (1800s)
mathematical treatment of “preferred outcomes”

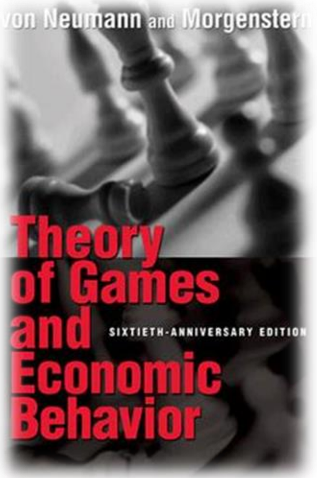
✓ Decision theory:= Utility + Probability (1900s)

Game Theory: Von Neumann (1944)
"the classic work upon which modern-day game theory is based."

Operations research: WW II

Markov decision processes: Richard Bellman (1957)

Satisficing: Herbert Simon (1978 NP)
making decisions that are “good enough”



Introduction of an agent for intelligence

Foundations of AI

Philosophy

Mathematics

Economics

Biology

Psychology

Control Theory

Computer Eng.

Linguistics

Action requires conclusion := artefact

✓ Antiquity : Tools for computations

Data recording: knotted strings (BCE 4000)
First calculator: abacus (2500 BCE)
Software engineering: Sanskrit grammar (~Turing machine) (500 BCE)
Binary code: Chandaḥśāstra (200 BCE)
Sequence Control: Heron of Alexandria (30 CE)
…
Automata: “Book of Ingenious Devices”, memory, feedback control, delays
…

✓ Renaissance : Tools for computations

Mechanical calculators, slide rule, punched cards …

Introduction of an agent for intelligence

Foundations of AI

- **Philosophy**
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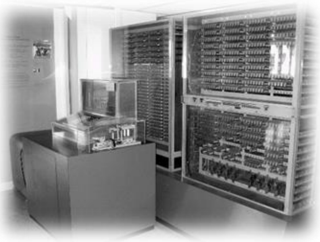
- **Computer Eng.**
- **Linguistics**

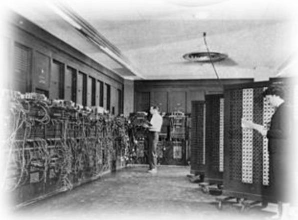
Action requires conclusion := artefact

✓ Operational, Programmable, Computer: Z-3



Konrad Zuse, Germany (1940): code and data stored on punched film
invented floating point numbers
first high level language *Plankalkül*

✓ Electronic, Digital Computer: ENIAC



US Army, 1945: calculate artillery firing tables, thermonuclear weapons
Performance : 30 sec./calculation << 20 hours (human) => x2400 fold

- Computational performance doubled every 18 months (2005)
- Massive parallelism ========> "nature-inspired" architectures

It is rather as if philosophers were to proclaim themselves expert explainers of the methods of stage magicians, and then, when we ask how the magician does the sawing-the-lady-in-half trick, they explain that it is really quite obvious:

The magician doesn't really saw her in half; he simply makes it appear that he does.

"But how does he do *that*?" we ask.

"Not our department," say the philosophers.

Daniel Dennett 1984

Data Driven Engineering

- ✓ Data intensive (driven) science / engineering is not new
  fertile crescent / Nile water regimes, astronomy …
- ✓ **Synergy**: Simulations ⇔ Experimental Discovery

Questions to Ponder

- ❑ Can the observation be generalized?
- ❑ What features are needed to be modeled?
- ❑ Can I model the desired features?
- ❑ What is the data I need to represent the feature?
- ❑ Can I access / collect that data?
- ❑ What is my objective function?
- ❑ How the model will be used? Who is the „customer“?

Book of Fixed Stars

Dunhuang Star Chart

La Silla Observatory

Data Driven Engineering: Data and Model

Karlsruhe Institute of Technology

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Data

- Observation >> Data
  - Generalizability (deep data)
- Big data vs. smart data
- Types of the data
  - numerical, categorical, ordinals
  - temporal correlation
- Dimensionality
- “Labelled” data

Data Driven Engineering: Data and Model

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fertile crescent / Nile water regimes, astronomy …

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Model

- Physical system => Math. => Physical context
- Model = **f**(Data)
  - << 5000+ years of cultivation: "recipes"
- What are the inputs and outputs?
  - What is easy to measure /calculate?
- How am I going to judge the outcome?
- Model developer:
  - What questions to be answered
  - What are properties of a good model?

DDE: Dynamical Systems

Discovery // Characterization // Simulation

Parameters

$$f(x, t, \alpha, \beta)$$

state

Temporal Dependency

Dynamics of State x

MODELING THE OBSERVATION

First Principles Eq.

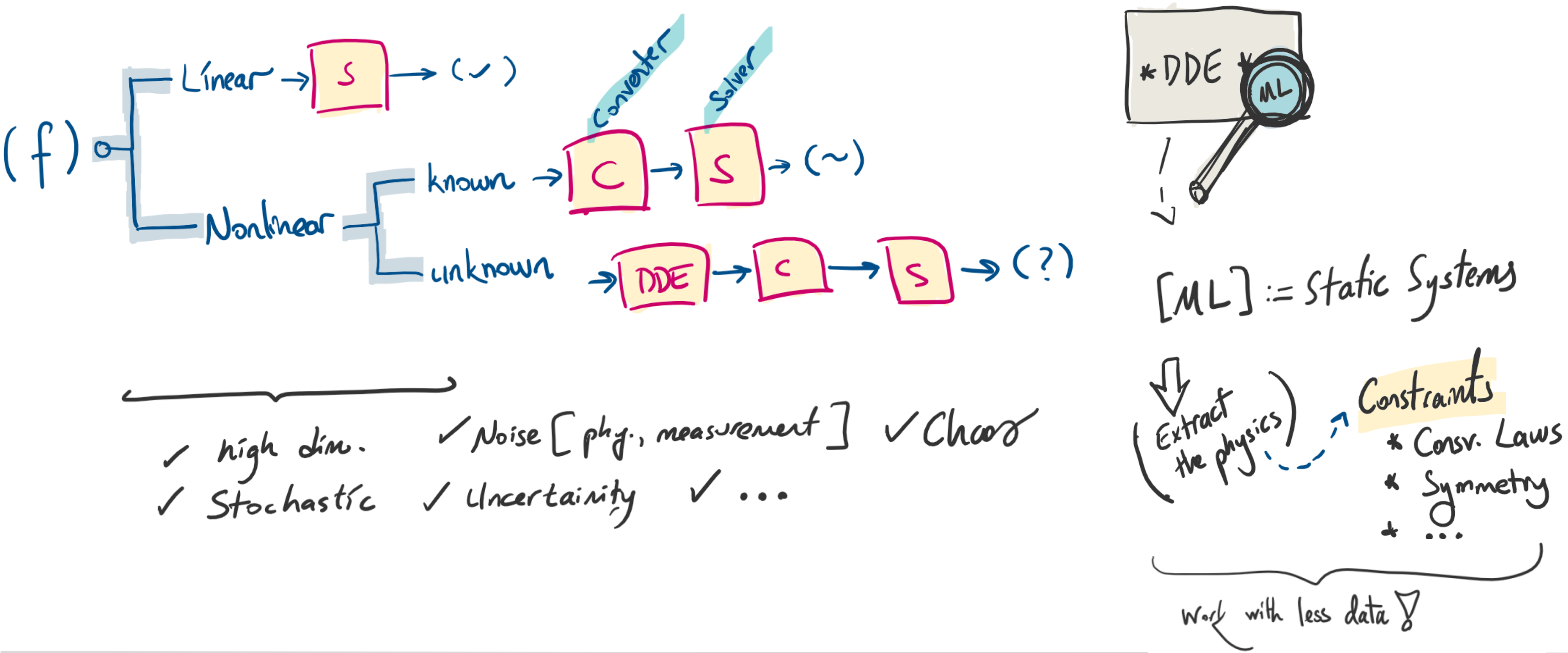
"Theory of Everything"

"Data Driven Models"

DDE: Dynamical Systems

Discovery // Characterization // Simulation

Karlsruhe Institute of Technology



DDE: Dynamical Systems

Discovery // Characterization // Simulation

❑ Objective << Discovery // Characterization // Simulation

❑ Methods

Machine Learning algorithms

- ✓ Classification
- ✓ Regression
- ✓ Clustering
- ✓ NN and Deep learning
- ✓ …

❑ Goals

- ✓ Future state predictions
- ✓ Design and optimization
- ✓ Process control
- ✓ Hypothesis generation
- ✓ …

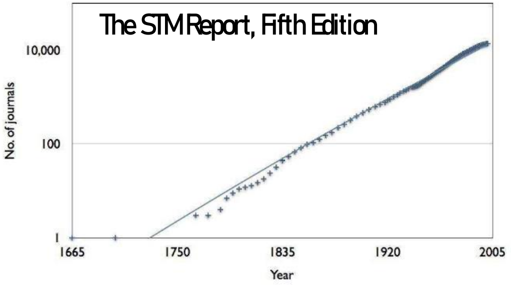
Why is it a good time: Data

Tools

- Development in the sensing technologies: Data
- Computational power: Data
- Data storage, transfer and processing: Data
- Accessible, high performance ML algorithms: Models
- Post processing tools: Data, models

Data:

- ❑ 33,119 active journals (42,491)
- ❑ Scopus: ~22,000 Journals
  - 69 million core records
  - 2.6 M papers added in 2018
  - 5 papers / min.



Why is it a good time: Model

Tools

- Development in the sensing technologies: Data
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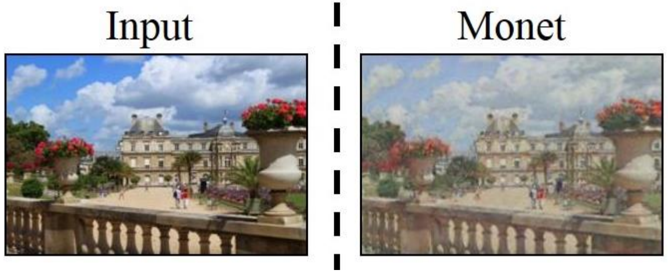
- Post processing tools: Data, models

Models:

- ❑ Deep Learning (2006) (1962)
- ❑ GANs (2014)
- ❑ AlphaZero (2017)
- ❑ Transformers (2017-)
- ❑ MuZero (2019)



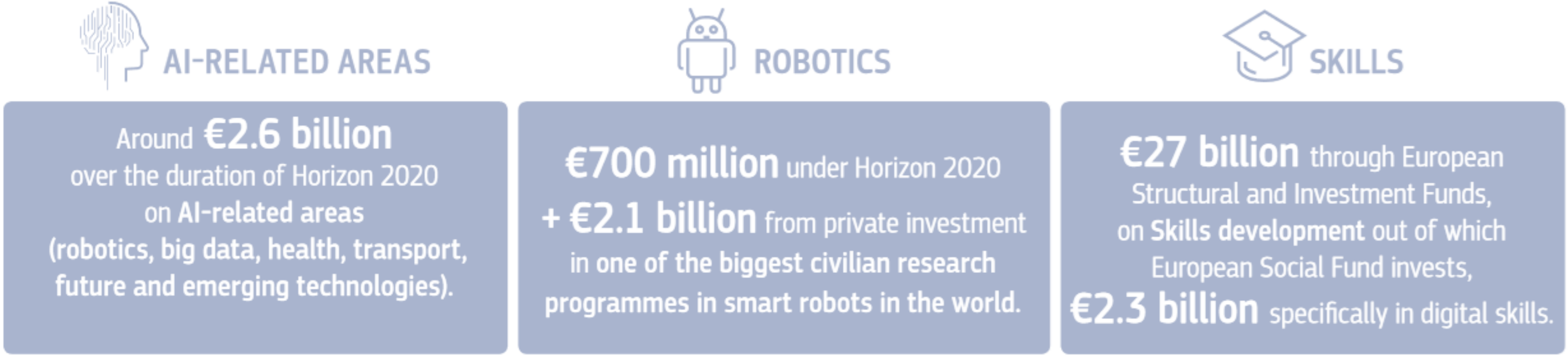
junyanz.github.io/CycleGAN/

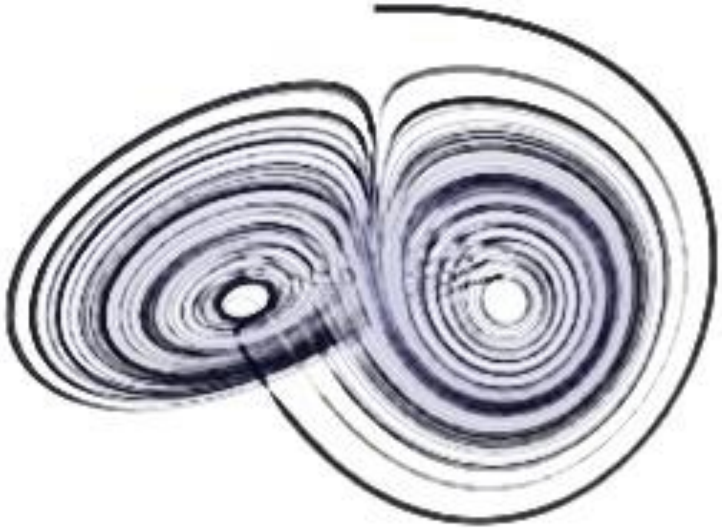
Why is it a good time = Support

- AI Investment (private, 2016):
  - Europe: ~ € 3 billion
  - Asia: ~ € 8 billion
  - N. America: ~ € 15 billion

Europe Investment: 2014-2020

- 2018-2020 R&D Investment : €20 billion
- After 2020:
  - ✓ €20 billion per year on AI
  - ✓ €1 billion per year via Horizon Europe





Examples

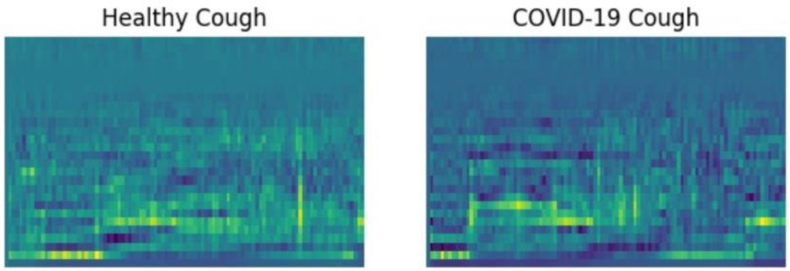
COVID-19 Artificial Intelligence Diagnosis using only Cough Recordings
IEEE Open Journal of Engineering in Medicine and Biology, 30.10.20

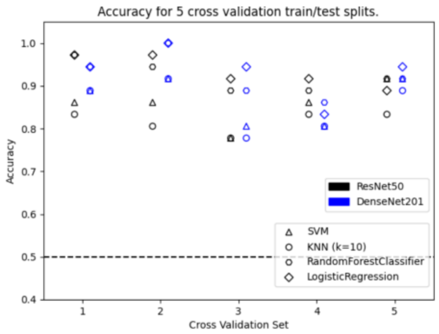
- ❑ Prof. Sanjay Sarma, MIT AUTO-ID LABORATORY
  - ❑ coined the term Internet of Things, ~ 300 publications, ~13000 citations

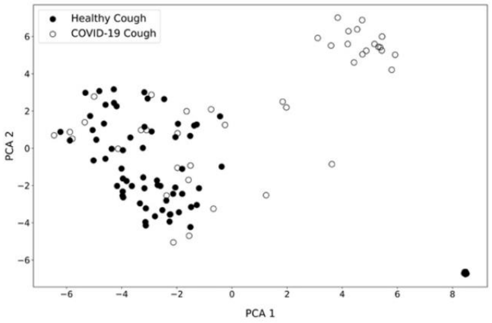
- ❑ ML trained on cough phone recordings
  - ❑ Aim: data on 150 patients and 3000 contacts
  - ❑ Initially: < 200

- ❑ Audio recordings can be used to diagnose pneumonia

"Until we have a sizable and longitudinal sample database, we cannot be sure how many useful tests a COVID-19 detection algorithm can extract from sound signals"





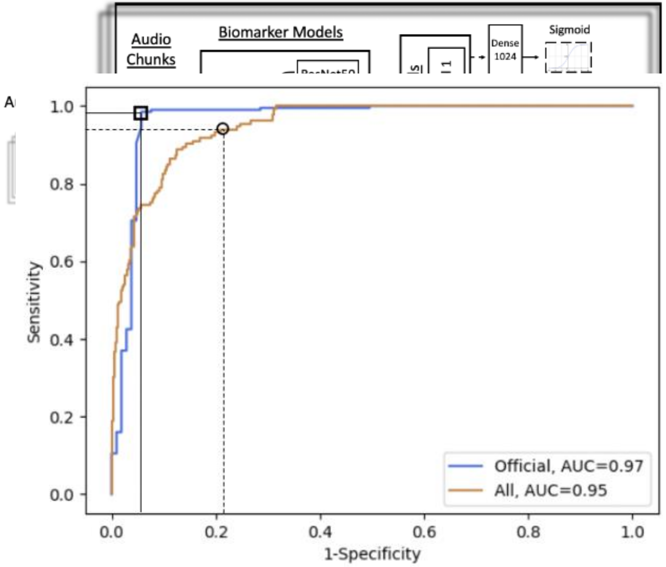


COVID-19 Artificial Intelligence Diagnosis using only Cough Recordings
IEEE Open Journal of Engineering in Medicine and Biology, 30.10.20

- ❑ Second Paper: 5 Full Text Views!
- ❑ 5,320 subjects (4256/1064)
- ❑ Convolutional Neural Network (CNN) based architecture
- ❑ COVID-19 sensitivity of 98.5%
- ❑ Specificity of 94.2% (AUC: 0.97)
- ❑ 9 commercially available: 40-86% sens.

"there are cultural and age differences in coughs, future work could focus on tailoring the model to different age groups and regions of the world".

- Mount Sinai and White Planes Hospitals in the US
- Catalan Health Institute in Catalonia
- Hospitales Civiles de Guadalajara in Mexico
- Ospedale Luigi Sacco in Italy

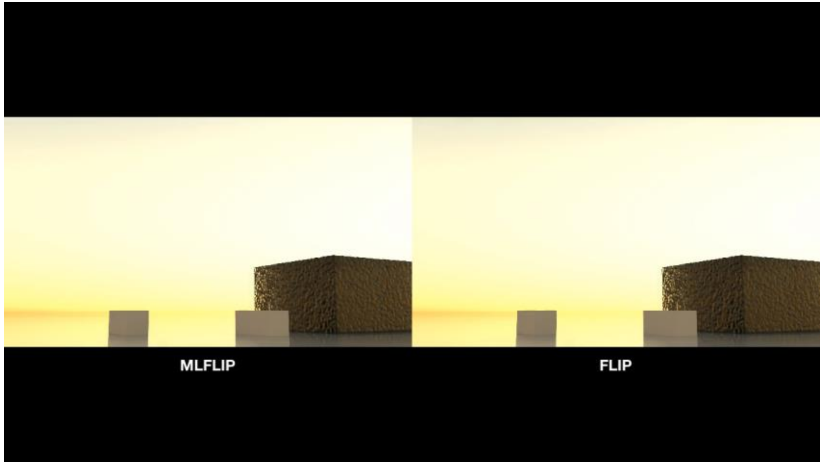


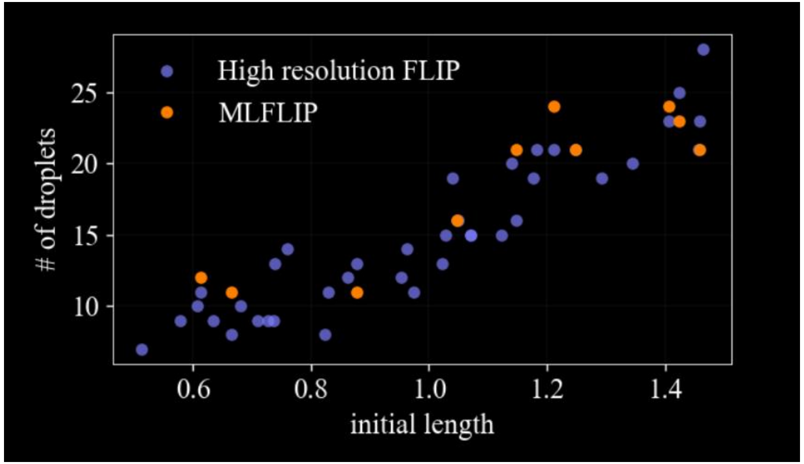
- Sentiment Speech classifier
- respiratory tract get altered with respiratory infections

Data Driven Splash Modeling

Liquid Splash Modeling with Neural Networks

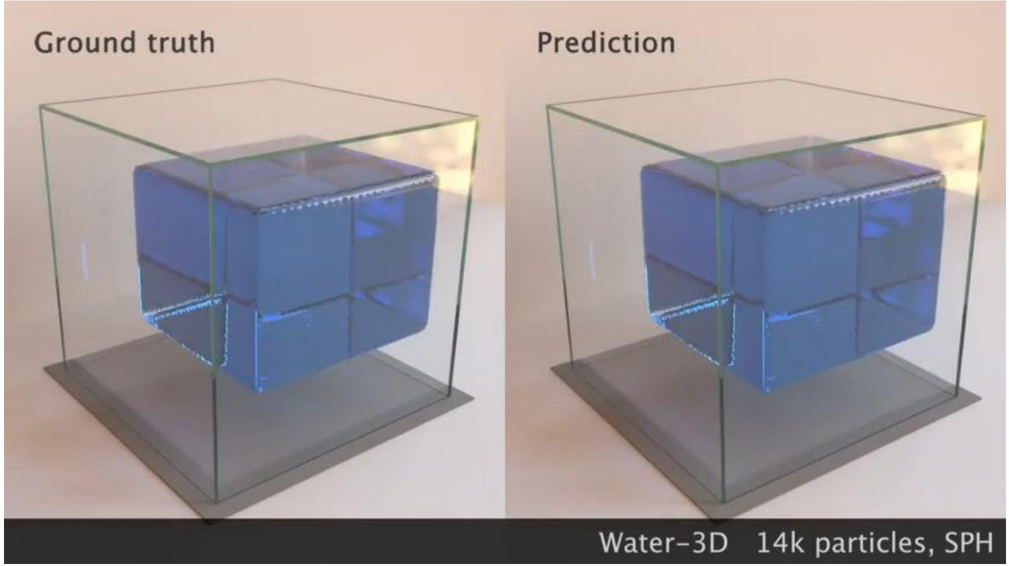
ERC Starting Grant 637014





- ❑ Detailed splashes for liquid simulations with neural network
- ❑ fluid-implicit-particle (FLIP) algorithm (PIC)
- ❑ Learning the formation of small-scale splashes from physically accurate simulations (~x10 faster)

Simulate Complex Physics with Graph NN

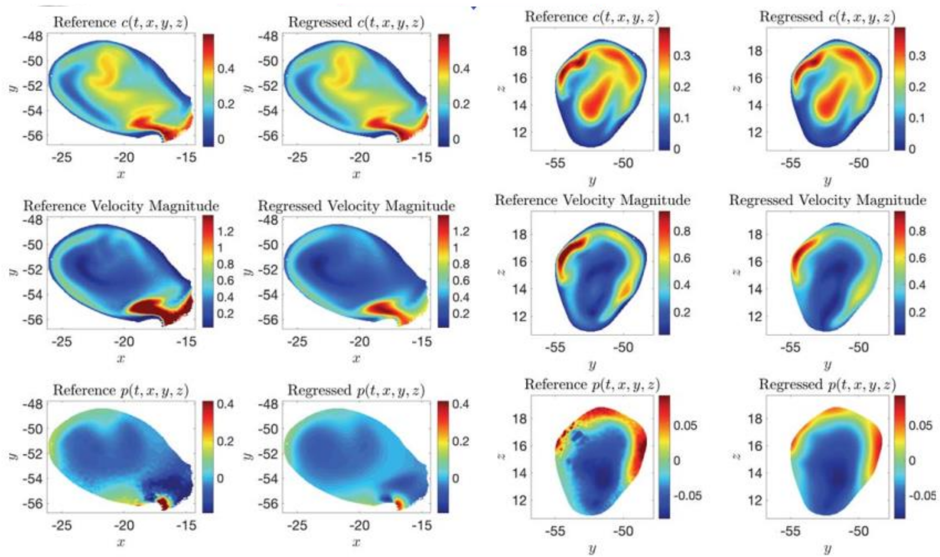


- ❑ Graph Nets library of DeepMind
- ❑ Autoencoder (TF)

Experimental domain	N	K	1-step ($\times 10^{-9}$)	Rollout ($\times 10^{-3}$)
WATER-3D (SPH)	13k	800	8.66	10.1
SAND-3D	20k	350	1.42	0.554
GOOP-3D	14k	300	1.32	0.618
WATER-3D-S (SPH)	5.8k	800	9.66	9.52
BOXBATH (PBD)	1k	150	54.5	4.2
WATER	1.9k	1000	2.82	17.4
SAND	2k	320	6.23	2.37
GOOP	1.9k	400	2.91	1.89
MULTIMATERIAL	2k	1000	1.81	16.9
FLUIDSHAKE	1.3k	2000	2.1	20.1
WATERDROP	1k	1000	1.52	7.01
WATERDROP-XL	7.1k	1000	1.23	14.9
WATERRAMPS	2.3k	600	4.91	11.6
SANDRAMPS	3.3k	400	2.77	2.07
RANDOMFLOOR	3.4k	600	2.77	6.72
CONTINUOUS	4.3k	400	2.06	1.06

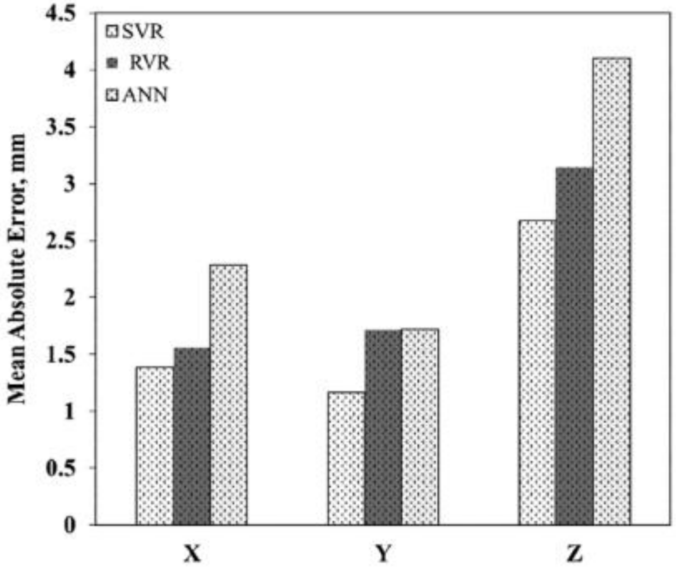
- ❑ Simulate wide range of physical systems in which fluids
- ❑ Generalize to larger systems / longer time scales

Other Recent Examples (TF)



NN Flow Visualization
c(t, x, y, z) => v, p

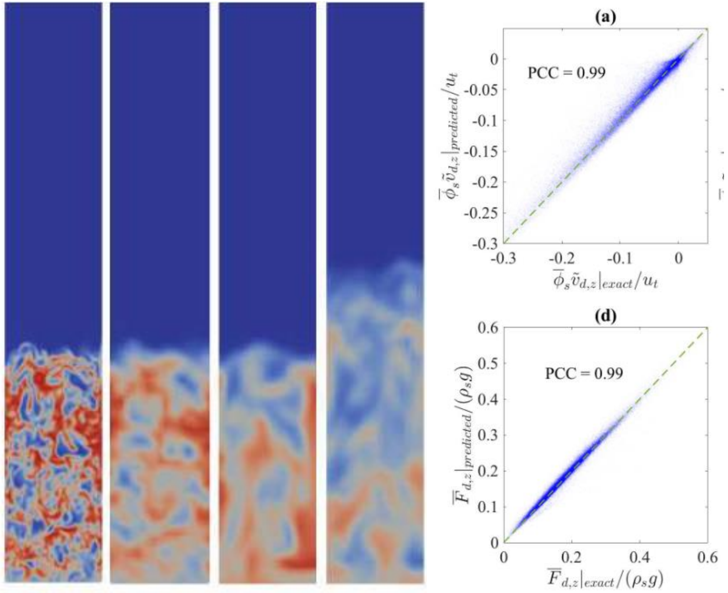
Science 367, 1026–1030 (2020)



NN Radioactive particle tracking position reconstruction

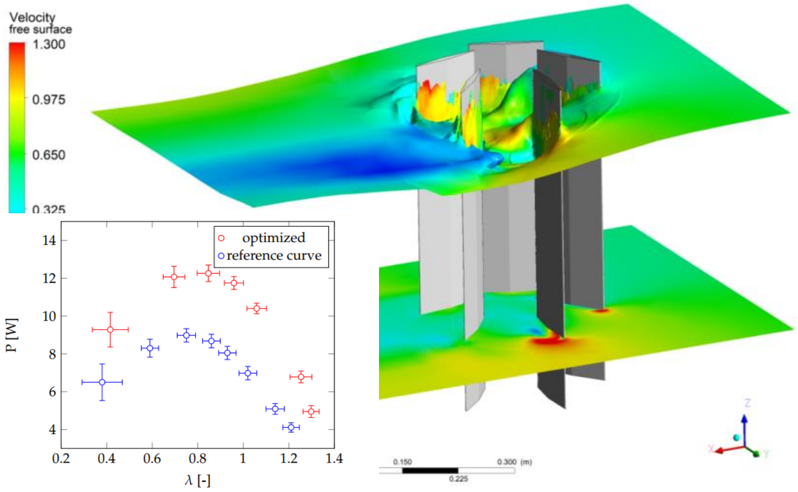
AIChE J. 2020;66:e16954

Other Recent Examples (TF)



Drag Models for Fluidized Beds

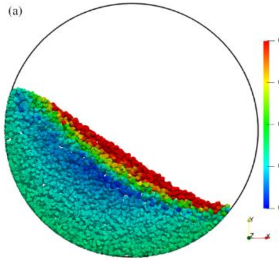
Chem. Eng. Sc. https://doi.org/10.1016/j.ces.2020.116235

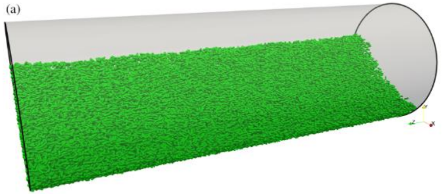


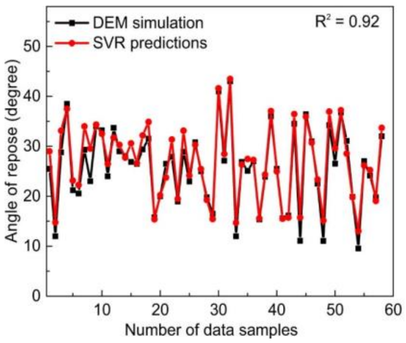
Performance Optimization of a Kirsten–Boeing Turbine

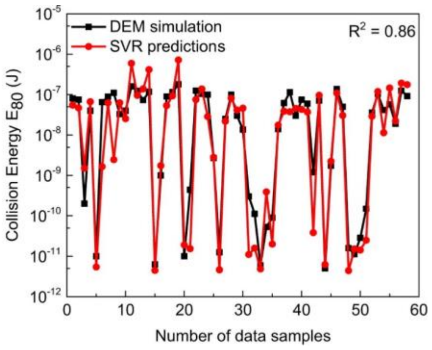
Energies 2019, 12, 1777 ; doi:10.3390/en12091777

Other Recent Examples (TF)



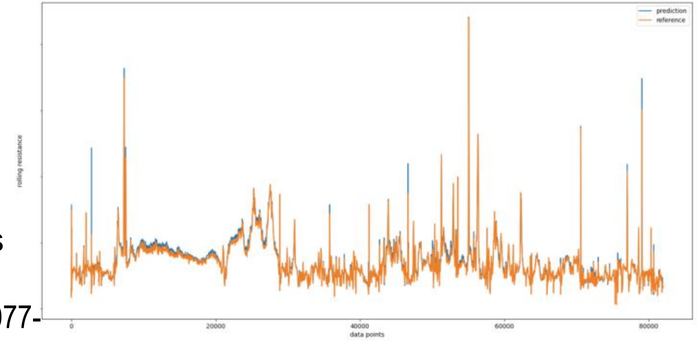




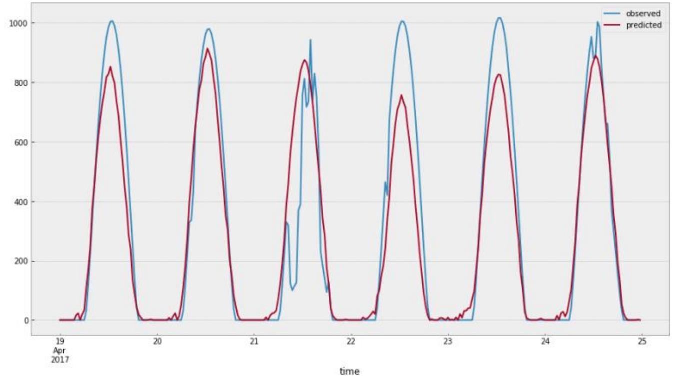


Particle flow in rotating drums
10.1016/j.ces.2020.116251

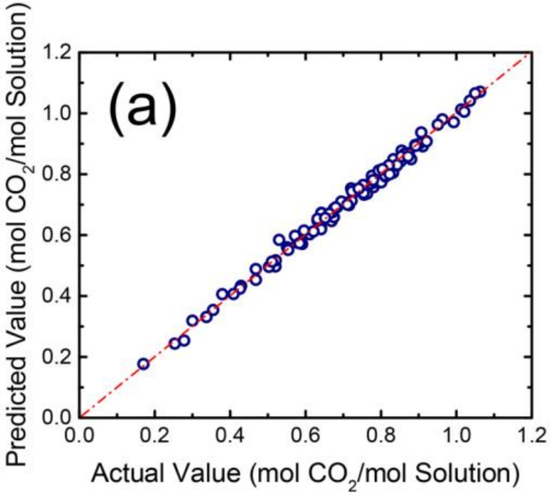
Tire Energy Loss Prediction
10.1007/978-3-030-38077-9_216



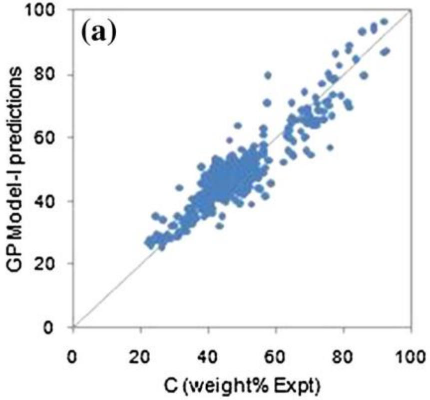
Forecasted solar Irradiance
10.1109/IECON.2019.8926801



Other Recent Examples (TF)

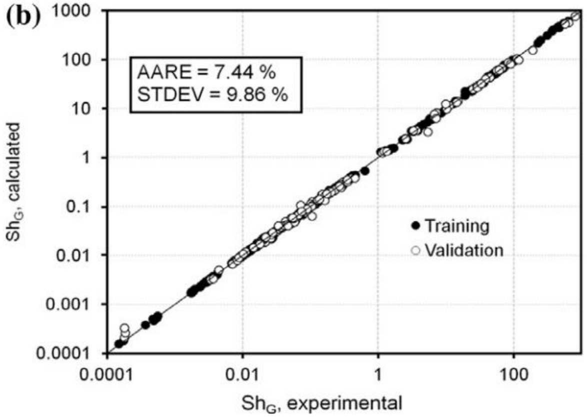


CO_2 thermodynamic properties in solution
Journal of CO_2 Utilization 26 (2018) 152–159



UA from PA for
solid biomass fuels

DOI 10.1007/s13198-014-0324-4



Transport models for trickle
bed reactors

Chemical Engineering Journal 207–208 (2012) 822–831

Others…

- Energy landscape predictions
- Laminar burning velocities of Syngas-Methane mixture
- Ignition Process
- Optimal process routes in plant design

- Material design
- MD simulations
- Physical property estimations
- Phase Equilibrium Predictions

- Learning to predict chemical reactions
- Clustering method applied to reaction mechanisms
- Mass transfer rate predictions in reactors

- Ball bearing fault diagnostics
- Abnormality detection in air conditioning systems
- Gear Diagnosis and prognosis
- Detection of crack/unbalancing in a rotor system
- Fatigue stress predictions in aircrafts

- Laser micro-grooving optimization
- Welding robot systems

- Pose detection
- Smart farming / crop identification

- Hypothyroidism / hyperthyroidism detection
- Cancer Malignancy Classification
- Arrhythmia detection

Summary

- ❑ Flow of the lecture is described.
- ❑ Keywords and key figures of AI is introduced. Feel free to explore!
- ❑ The DDE aproach is present.
- ❑ A glimpse of the ML in the current SoA is presented.
- ❑ Note: Images are taken from Wikipedia if not stated otherwise.

Reminders

- ❑ Register on ILIAS
- ❑ Survey and pool on ILIAS: Participate today!
- ❑ References will be updated on the forum (ILIAS).
- ❑ Open up your (dummy) account and link it to Colab (colab.research.google.com)
- ❑ Look up forum for local installation

Machines will be capable, within twenty years, of doing any work a man can do.

Herbert Simon, 1965

***

From three to eight years, we will have a machine with the general intelligence of an average human being.

Marvin Minsky, 1970

***

"The most fruitful areas for the growth of the sciences were those which had been neglected as a no-man's land between the various established fields."

Norbert Wiener, 1948

Additional Notes

Interpreting the Intelligence-I

Human-like Acting:

- ❑ Performance
- ❑ Functions requiring intelligence
- ❑ Turing Test

““If a machine is expected to be infallible it cannot also be intelligent.”

- ✓ NLP: Ability to communicate
- ✓ Knowledge representation (context)
- ✓ Automated reasoning: draw conclusions
- ✓ ML: Detect, adapt and extraploate
- ✓ Vision & Robotics

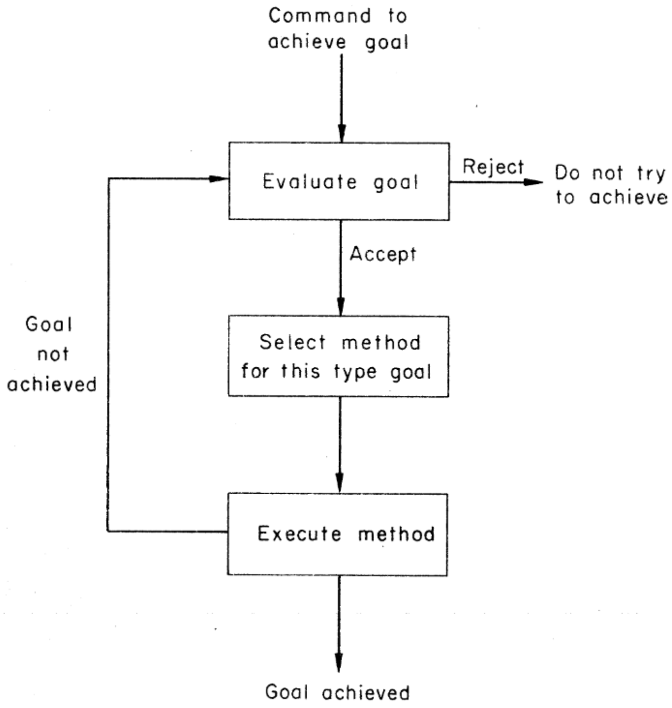
Underlying Principles

Interpreting the Intelligence-II

Human-like thinking:

- ❑ Decision Making
- ❑ Problem Solving
- ❑ Learning
- ❑ Machines with minds: literally!

- ✓ How humans think? (Cognitive Sci.)
- ✓ Trace of its reasoning steps is similar to those humans follow
- ✓ General Problem Solver (GPS), 1959



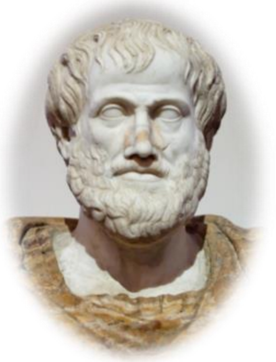
Aristotle's algorithm

Interpreting the Intelligence-III

Rational thinking:

- ❑ Computational models
- ❑ Mental faculties
- ❑ Laws of thought

All men are mortal.
Socrates is a man.
Therefore, Socrates is mortal.



- ❑ Syllogism: **deductive reasoning** to arrive at a conclusion
- ❑ Logicist tradition within artificial intelligence
  - Informal => formal conversion
  - Uncertainity

Interpreting the Intelligence-IV

Rational Acting:

- Intelligent agents
- Intelligent behavior in artifacts
- rational-agent approach

'An attempt at a new analysis of the mortality caused by smallpox and of the advantages of inoculation to prevent it.'

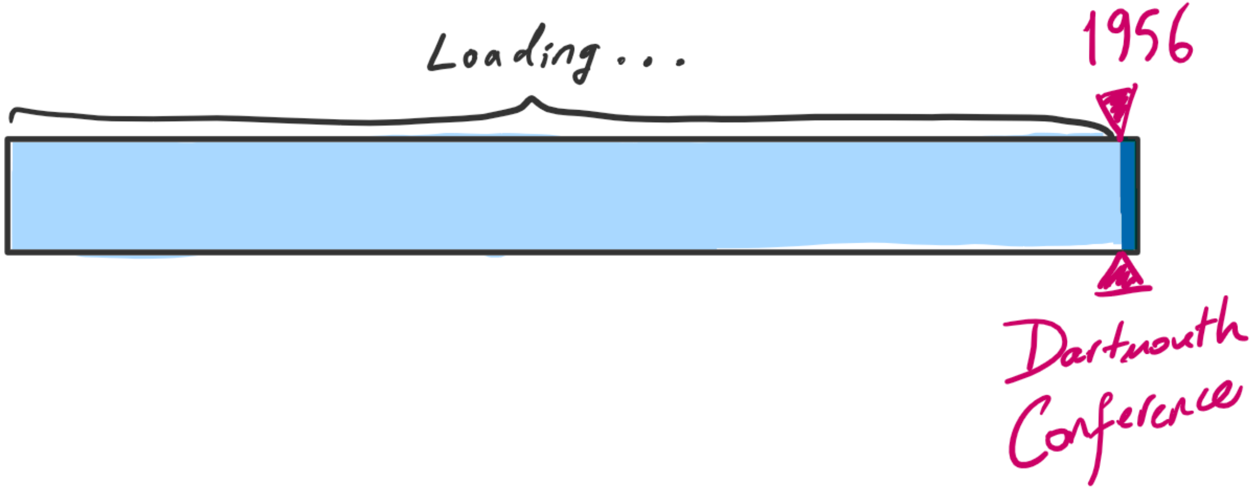
Daniel Bernoulli, 1766

- A **rational agent** is one that acts so as to achieve the **best** outcome or, when there is uncertainty, the **best expected outcome**.

– Perfect rationality is not feasible in complicated environments

✓ Limited rationality: acting appropriately when there is not enough time to do all the computations.

Birth of AI



Birth of AI

I | II | III | IV

I. Great Expectations (1950s – 1970)

- GPS
- LISP Language
- Games
- "Microworld" Simulations ...
- Perceptron & NN
- Genetic Alg.

II. Facing the Reality (1960 - 1970)

- NLP ⇒ Sputnik (1957)
  - ⇒ Translation of Papers
  - ⇒ "Sprit is willing but the flesh is weak."
  - → Vodka is good but meat is rotten."

All funds cancelled !?

→ Tractability: Working in "microworlds" Fails in practice. [a few dozens]

III. Specialization: Knowledge-based Approach (1970 - 1980)

- Special purpose rules [Cookbook Recipes]

→ Expert Systems

IV. AI is cool again: Attracting Industry (1980s →)

⇒ 1980: A few million $
1988: Billion $

✓ Expert Systems
✓ Vision
✓ Robotics

✓ Specialized hardware
✓ Spec. Software

History of A.I. at a glance

Karlsruhe Institute of Technology

→ AI Adopts Scientific Method (1987)

× Brand-new ideas & theories

× intuition

↳ Builds upon existing work!

↳ Exp. Evidence

2000s

* Large Datasets become available.

* "Algorithm" is the key.

* Data is good enough?

1990s

→ Intelligent Agent ⟺ "Internet"

• "-bot" suffix

× HLAI: Human Level AI; Some key figures are not happy?

Artificial General Intelligence..