

Fundamentals of Machine learning for and with engineering applications

Enrico Riccardi¹

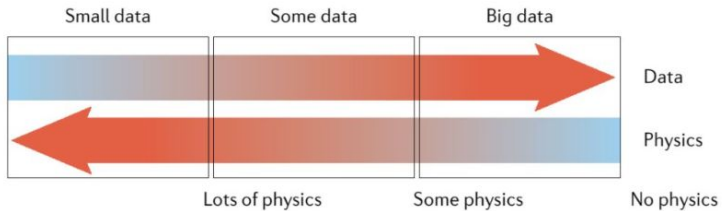
Department of Energy Resources, University of Stavanger (UiS).¹

Jan 16, 2025



- 1 Recaps: Data concepts, Data types and Models
- 2 Descriptive and Predictive statistics
- 3 Simulations
- 4 Statistics, Machine learning or Artificial intelligence?
- 5 Metadata

Data vs Physics



Uncertainty

- Def 1: Not knowing if an event is true or false. (Useful)
- Def 2: Things that cannot be measured. (Not useful)

Probability is how Uncertainty is quantified!

- Clarity test
- Assign a number between 0 and 1 to our degree of belief
- Error definition

Sentence also good for fortune cookies

Uncertainty is the only certainty

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Uncertainty and Probability

Random quotes

- Probability: there is not science more worthy in our contemplations nor a more useful one for admission to our system of public education
- The theory of probabilities is at the bottom of nothing but common sense reduced to calculus.

What is Statistics

Clarity test. Beer drinker?

Rain in Stavanger?

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Data properties

1 D

logs

2 D: maps

Quite limited but great for visualization

3 D

3d maps, seismic cubes. More informative, mostly ok in digital formats.

4 D

Trajectories

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Data realm

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Types of data

- Categorical / Nominal (classes)
- Categorical / Ordinal
- Continuous / Interval (e.g. Celsius)
- Continuous / Ratio
- Discrete: binned/grouped data
- Hard data: direct measurements
- Soft data: indirect measurements, very uncertain
- Primary data: variable(s) of interest
- Secondary data: descriptors
- Collective variables
- Latent variables

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Descriptive and Predictive statistics

Estimation

- Process of obtaining the best value or range of a property in an unsampled location
- Local accuracy takes precedence over global spatial variability
- Not appropriate for forecasting

Inference

- Predict unseen samples given assumptions about the population
- Test with a pre-trained model (ML definition)
- Generality versus Accuracy

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Variables and Features, Labels and Instances

Population

Exhaustive, finite list of properties of interest over area of interest.

Generally the entire population is not accessible

Samples/experiments/instances

The set of values and location that have been measured.

How many experiments are needed?

Features

The values to be measured for each sample/experiment/instance.

How many features are needed?

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Variables and Features, Labels and Instances

Predictors = input variables, X_1, \dots, X_M

Response = output variables

Error

Deviation from ... exact value (or expected value, mean value, trend...?)

Errors without definitions are just numbers.

Predictor and Response Features

Given a model $Y = f(X_1, \dots, X_M) + e$

!Here and error! But is it even an error?

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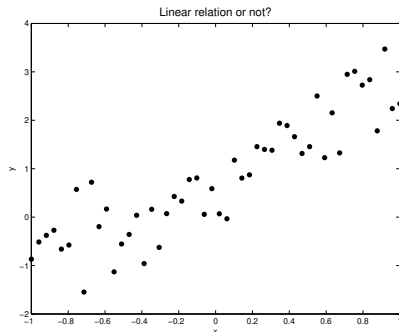
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Finding a suitable model

Soft modeling is in most cases based on **multivariate statistical methods**. Many of these methods may be viewed as sophisticated ways of performing curve fitting to data.



What would be the best model?

- Straight?: $y(x) = ax + b$
- Parabolic?:
 $y(x) = ax^2 + bx + c$
- Trigonometric?:
 $y(x) = a\sin(x) + b\cos(x)$

Uncertainty Modeling

Given a model, Generate multiple simulation to represent uncertainty

- Realizations: for the same input parameters, different random numbers.
- Scenarios: different input parameters.

Sampling representative.

Random sampling

Each item of the population has an equal chance of being chosen.

- Very expensive
- Mostly not interesting
- Gives some global properties

Bias sampling

Selection of data is (arbitrarily) distorted

- Sample probability bias has to be corrected for
- Might not capture the global picture

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Cognitive biases

- anchoring: The first bits are over-considered
- availability: over-estimating the importance of info
- bandwagon: P increases with the number of people holding a belief
- blind spot: not seen biases
- choice supporting: commitment/decision dependent
- clustering illusion: seeing patterns in random events
- confirmation bias
- conservatism bias
- Recency bias
- Supervision bias
- Many many more!

Bias DO NOT cancel out! They sum up (or multiply?)

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Simulations

Process of obtaining one or more values of a property

- Improved Global accuracy
- Better property distributions

Why simulations then?

- We need to capture the full distribution of properties, extremes matter!
- We need more realistic models.

Why not?

- High dimensionality level
- Computationally expensive
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- Constitutive equations need to be rather accurate.

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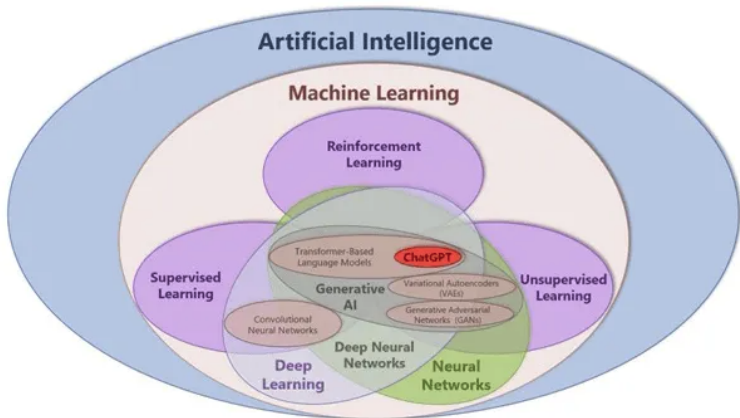
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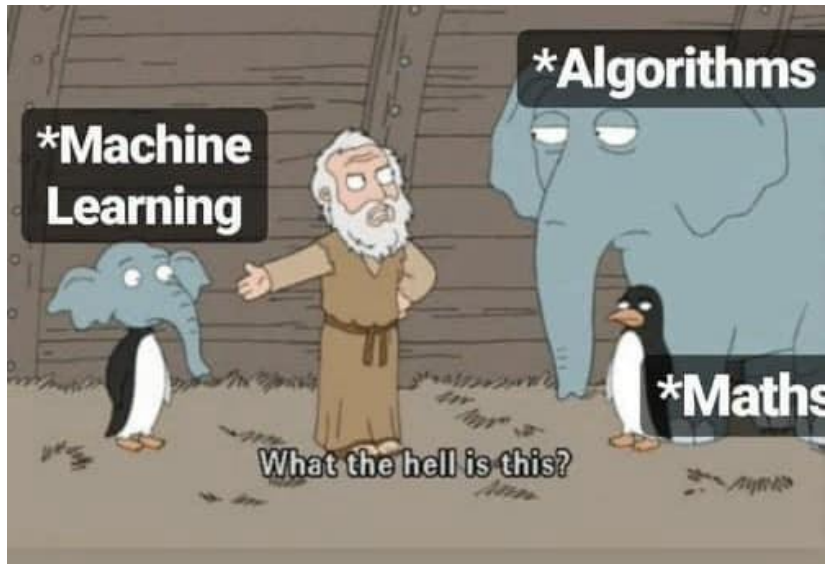
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Statistics, Machine learning or Artificial intelligence?

What is the main difference between the three fields?



How Machine Learning Started?



Let's start from the definition

- Statistics (origin "description of a state/country") is the discipline that concerns the collection, organization, analysis, interpretation, and presentation of data.
- It is conventional to begin with a statistical population or a statistical model to be studied. Populations can be diverse groups of people or objects such as "all people living in a country" or "every atom composing a crystal".
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Definitions:

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- Machine learning (ML) is a field of study in artificial intelligence concerned with the development and study of statistical algorithms that can learn from data and generalize to unseen data, and thus perform tasks without explicit instructions. [WIKI]
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The loss function is the actual engine in machine learning.

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And more definitions:

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Data properties

- All starts from data: what are data-properties?
- Are there such things as good data and bad data?

Main lesson (Exam question)

- Data **DO NOT** always have value.
- TRASH in TRASH out

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Metadata properties

Data without metadata are just numbers (i.e. if they are integers, they are still good to play lottery)

Metadata can be pretty much anything. Depending on the application, we can distinguish between:

- 1 Descriptive : used for discovery and identification. It includes elements such as title, abstract, author, and keywords.
- 2 Structural : describe how compound objects are put together. It describes the types, versions, relationships, and other characteristics of digital materials.
- 3 Administrative : to help manage a resource, like resource type, permissions, and when and how it was created.
- 4 Reference : to indicate the information about the contents and quality of statistical data.
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They are a must for:

- Code repositories
- Data repositories

Please click on the link and explore. Those are just some of the open (scientific) repositories. The aim/hope is to allow people to extract information. How to make value from that information... is another story.

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MetaData for sharing and re-use

More considerations:

- Metadata is more and more important in a digital open world.
- Researchers and automatic algorithms would benefit from importing data directly.
- FAIR research is an important part of Open Science revolution (Findable, Accessible, interoperable, Reusable)
- New applications, business, discoveries can be thus enabled.
- ChatGPT, Bard, Gemini, and all the LLMs are functional only thanks to this!

Super controversial

- Who would be responsible for them then?
- What is the advantage for who releases the data?
- Who gets the money for what?
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- Researchers and automatic algorithms would benefit from importing data directly.
- FAIR research is an important part of Open Science revolution (Findable, Accessible, interoperable, Reusable)
- New applications, business, discoveries can be thus enabled.
- ChatGPT, Bard, Gemini, and all the LLMs are functional only thanks to this!

Super controversial

- Who would be responsible for them then?
- What is the advantage for who releases the data?
- Who gets the money for what?
- Copyright for data and/or for data processing?

MetaData for sharing and re-use

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- Norwegian offshore directorate
- Norway Statistics
- World statistics
- Code repositories
- Data repositories